2010 Functional and Structural Nanomaterials: Fabrication, Properties, Applications and Implications: Synthesis of Nanomaterials III

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Nanomaterials Committee
Program Organizers: David Stollberg, Georgia Tech Research Institute; Nitin Chopra, University of Alabama; Jiyoung Kim, University of Texas - Dallas; Seong Jin Koh, University of Texas at Arlington; Navin Manjooran, Siemens Corporation; Ben Poquette, Keystone Materials; Jud Ready, Georgia Tech

Wednesday AM Room: 214
February 17, 2010 Location: Washington State Convention Center

Session Chair: Seong Jin Koh, University of Texas at Arlington; Navin Manjooran, Siemens Corporation

8:30 AM Introductory Comments

8:35 AM
Effect of Milling Parameters on the Structural Stability of Isothermally Heat Treated Nanostructured Al-2.7at. %Ni Mechanically Alloyed Eutectic Powders: *Hanadi Salem*[1]; Mohy Eldin Raged[1]; [1]American University in Cairo

In the current research optimum milling parameters and energy domains for the synthesis of Nanocrystalline Al-2.7 at.%Ni eutectic alloy was determined. Effect of milling parameters on the eutectic platelets morphology of Al3Ni was investigated. Structural stability before and after isothermal heating at temperatures higher than the recrystallization temperature was investigated using a differential scanning calorimeter. TEM and SEM were employed for the characterization of the structural evolution. The average stored energy increased with increasing the milling time, ball-to-powder ratio (BPR) and rotation speed (RPM). The average stored energy recorded for the powders milled at 200RPM for 40 hrs was 16.571 and 42.39j/g for the 5:1 and 10:1 BPR, respectively. The variation in dislocation densities was calculated for the mechanically alloyed powders before and after isothermal heating.

8:55 AM
Influence of the Dispersion Mechanism of Nanostrucutred Al50Ni50 Intermetallic Compound in Al-Matrices on the Consolidation Behavior and Structural Stability: *Hanadi Salem*[1]; Abdel Hamid Abdel Hamid[1]; [1]American University in Cairo

Fabrication and processing of Aluminum reinforced AlNi intermetallic MMCs with 0, 5, 10% volume fractions was carried out. 99.7% purity Al powder with mean particle size of 15 μm was mixed with mechanically alloyed nanostrucutred AlNi using either regular mixing or mechanical milling. The AlNi phase was fully formed after 12hrs of milling time, while prolonged milling for 31hrs resulted in a significant change in the powder morphology and produced nanopowders about 2μm in average size and 18nm crystallite size. The mixed powders were consolidated via a combination of cold pressing followed by hot extrusion at 480°C for 1hr using 4:1 reduction ratio. Hardness and tensile properties of the extruded composite powders were characterized. Structural evolution of the milled composite powders was investigated before and after extrusion using optical microscopy and Field Emission Scanning Electron Microscopy. Energy Dispersive Spectroscopy was employed for mapping the Intermetallic dispersion distribution within the matrix.

9:15 AM
Fabrication of Aluminum Carbon Nanotube Composites Via High-Energy Milling: *Joseph Paras*[1]; Ryan Carpenter[1]; Deepak Kapoor[1]; Stephen Bartolucci[1]; Tony Zahrah[2]; Rod Rowland[2]; [1]U.S. Army ARDEC; [2]MATSYS Inc.

Aluminum-Carbon Nanotube systems are of great military interest in the field of high performance, lightweight structural materials. Traditional methodologies for fabricating these composites involve wet mixing through solvents or direct wetting of nanotubes with molten aluminum. The work presented in this paper will focus on producing composites using dry powder mixing methods. Mixtures of aluminum and multiwall carbon nanotubes (MWCNTs) were used to produce nanostructured composite powders via high-energy milling. These powders were then consolidated using an instrumented hot isostatic press (HIP), which allows for real-time monitoring of sample densification. This process minimizes the exposure of the nanostructured powder to high temperature, and as a result, the microstructure of the final product can be controlled. Imaging of the consolidated pieces show MWCNTs sandwiched between aluminum lamellae, which is evidence of the retention of the nanostructure imparted during the high-energy milling process.

9:35 AM
Studies on the Mechanical Properties of Al-Mg-SiO_2 Metal-Matrix Nanocomposite Synthesized by Mechanical Alloying: *Nikhil Balachander*[1]; Shashank Shekher[1]; Arun Naik[1]; Jatin Bhatt[1]; D.R. Peshwe[1]; [1]VNIT Nagpur

Mechanical Alloying using high-energy ball milling was employed to produce a metal-matrix composite powder of Al-Mg reinforced with amorphous silica particulate. Nano and submicron-sized silica particles embedded in an Al-Mg matrix were obtained. Four different compositions were chosen with varying magnesium content (0.5%, 1%, 2.5%,5% by weight). No new phases were found in mechanically alloyed Al-Mg-SiO_2 nanocomposite powder. X-ray diffraction analysis showed that magnesium dissolves into the aluminum matrix completely. It was also found that crystallite size decreased and lattice strain increased with progress in mechanical alloying. Scanning electron micrographs indicate a decrease in particle size via plastic deformation and fracture. The powders are compacted to pelletized form by Spark Plasma Sintering for evaluation of mechanical properties. The mechanical properties of this nanocomposite will be discussed with a focus on possible applications in the automotive industry.

9:55 AM Break

10:10 AM
Microstructures and Electrochemical Properties of Nanostructured Mg2Ni-Based Compound Containing Nb Additives: *Maryam Mohri*[1]; Seyed Farshid Kashani Bozorg[1]; [1]University of Tehran

High hydrogen capacity of Mg2Ni intermetallic compound has made it a candidate material for negative electrode of rechargeable Nickel Metal Hydride batteries. In the present work, two strategies were selected in order to improve its hydrogen absorption kinetic; synthesis of Mg2Ni-based nanostructured compound and modification of composition using Nb additives. High energy ball milling of binary and ternary powder mixtures (Mg1.75Nb0.25Ni and Mg2Ni0.75Nb0.25) was carried out. The effects of milling process and initial compositions on the microstructure milled products were studied employing X-ray diffraction and scanning and transmission electron microscopy. Also, electrochemical measurements of the nanostructured electrodes made from the milled product were measured using an automatic galvanostat. It was found that Mg1.75Nb0.25Ni has beneficial effect on the formation kinetic of Mg2Ni nanocrystallites. Electrode made from the 20h milled product using initial composition of Mg1.75Nb0.25Ni exhibited a high discharge capacity of ~600mAhg-1 and relatively longer discharge life.

10:30 AM
Influence of Using MgCO3 and MgO as Initial Materials on the Synthesis of Pure Nanocrystalline Forsterite Powder: F. Tavangarian[1]; R. Emadi[1]; *Ehsan Mohammadi Zahrani*[2]; [1]Isfahan University of Technology (IUT); [2]The University of British Columbia

Pure nanocrystalline forsterite (Mg2SiO4) powder was synthesized by mechanical activation technique followed by subsequent annealing. The starting materials were talc (Mg3Si4O10(OH)2), magnesium carbonate (MgCO3) and magnesium oxide (MgO) powders. To produce forsterite, two mixtures were prepared including talc and magnesium oxide (first mixture) as well as talc and magnesium carbonate powders (second mixture). First, both mixtures were milled by a planetary ball mill, and then annealed at 1000 °C and 1200°C for 1 h. Thermogravimetric (TG) analysis, X-ray diffraction (XRD) and SEM techniques were utilized to characterize synthesized powders. After 5 h of mechanical activation of the first mixture and subsequent annealing at 1000 °C for 1 h, pure nanocrystalline forsterite was synthesized with 40 nm particle size. A pure nanocrystalline forsterite with a particle size equal to 35 nm was obtained after 10 hr ball milling of the second mixture and subsequent annealing at 1000 °C for 1h.

10:50 AM
Development of Colloidal Single-Sized Photoluminescent Quanmtum Dots with Bandgap Photoluminescence: *Kui Yu*[1]; Michael Hu[2]; [1]National Research Council Canada; [2]Oak Ridge National Laboratory

Colloidal photoluminescent(PL) semiconductor nanocrystals have attracted significant attention over the past decade for both fundamental science and potential applications. For example, with tunable bandgap across the visible range (~400 nm to ~700 nm) of the electromagnetic spectrum, CdSe quantum dots(QDs) are of particular interest for the fundamental study of photophysics and have great potential in various applications including bio-imaging and bio-labeling. QDs are spherical semicondutor nanocrystals whose excitons are confined in three spatial dimensions, and can thus absorb and emit light size-dependently. Their optical properties, absorption and emission, are size-dependent. Therefore, one colloidal ensemble of regular QDs(RQDs) is fascinating, but with intrinsic difficulties to study: the variation in size leads to inhomogeneous spectral broadening, in addition to homogeneous spectral broadening. This presentation will address our recent advances in the synthesis of colloidal PL semiconductor QDs which are single-sized without inhomogeneous spectral broadening. The single-sized QDs are also termed as magic-sized QDs(MSQDs), including CdS, CdSe, CdTe, CdTeSe, and CdP.

11:10 AM Concluding Comments

Advances in Composite, Cellular and Natural Materials: Functional Composite Materials

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS/ASM: Composite Materials Committee
Program Organizers: Yuyuan Zhao, The University of Liverpool; David Dunand, Northwestern University

Wednesday AM — Room: 305
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Nik Chawla, Arizona State University; Katsuyoshi Kondoh, Osaka University

8:30 AM
Piezoelectric Smart Composites: Electromechanical Properties and Design Maps: *T Venkatesh*[1]; [1]Stony Brook University

Piezoelectric materials, by virtue of their unique electromechanical characteristics, have been recognized for their potential utility in many applications as sensors and actuators. However, the sensing or actuating functionality of monolithic piezoelectric materials is generally limited. The composite approach to piezoelectric materials provides a unique opportunity to access a new design space with optimal mechanical and coupled characteristics. An analytical model is developed to predict the complete elastic, dielectric and piezoelectric constitutive properties of a general piezoelectric composite, where the constituent phases are elastically anisotropic and piezoelectrically active. Furthermore, through finite-element modeling, a systematic methodology for quantifying the effects of piezoelectric characteristics (i.e., the poling direction), microstructural aspects (i.e., grain-size and phase volume fraction) and geometric features (i.e., size, shape, and distribution of the constituent phases), on the electromechanical response of piezoelectric composites is presented. Strategies for designing unique piezoelectric sensors with enhanced functionality in multiple directions are formulated.

8:50 AM
Ultrahigh Piezoresistive Effect Induced by Field Emission at Sharp Nano-Tips on the Surface of Spiky Spherical Nickel Powders: *Baoguo Han*[1]; Jinping Ou[1]; [1]Harbin Institute of Technology

The spiky spherical nickel powders with sharp nano-tips on their surface are dispersed into cement-matrix to fabricate nickel powder filled cement-based composites with ultrahigh piezoresistive response. The piezoresistive sensitivities of these composites to compressive stress and strain can reach to 0.19/MPa and 1932.0 respectively. This extremely high piezoresistive effect is attributed to the unique spiky surface morphology of nickel powers. Comparing to the normal smooth spherical nickel particles, the sharp nano-tip on the surface of spiky spherical nickel particles can induce field emission and tunneling effects, which leads to highly sensitive responses to compressive stress and strain.

9:10 AM
Extreme Piezoresistivity of Silicone/Nickel Nanocomposites for High Resolution Large Strain Measurement: Oliver Johnson[1]; *George Kaschner*[2]; Thomas Mason[2]; David Fullwood[1]; Tommy Hyatt[1]; Brent Adams[1]; Kevin Cole[1]; George Hansen[3]; [1]Brigham Young University; [2]Los Alamos National Laboratory; [3]Conductive Composites Company, LLC.

A Silicone/Nickel Nanostrand/Nickel Coated Carbon Fiber (Si/NiNs/NCCF) nanocomposite system has been developed for large strain and motion sensing applications. The response of this nanocomposite under various environmental conditions (i.e. temperature, humidity, pressure), strain rates, and cyclic loading has been studied. The useful strain range, resolution, strain rate sensivity, and fatigue properties of this system have been characterized. The Si/NiNs/NCCF nanocomposite was also adhered to various substrates which were subjected to tensile tests as well as four-point bending tests and traditional strain sensing techniques were used to verify the response of the nanocomposite gauges. This system was found to have an easily calibrated useful strain range of over 30% strain with better than microstrain resolution. These nanocomposite gauges serve as an inexpensive, easily applied after-market alternative to existing large displacement sensing techniques.

9:30 AM
Synthesis and Microstructural Evolution of Sic/Si3n4/Si2n2o Nitride Porous Ceramic Composites Processed via HYSYCVD: *Martin Pech-Canul*[1]; Jose Flores-Garcia[1]; [1]Centro de Investigacion y de Estudios Avanzados del Instituto Politecnico Nacional

The effect of using successive stages of infiltration and different atmosphere types on the microstructural evolution and physical properties of SiC/Si3N4/Si2N2O nitride porous ceramic composites was investigated. Composites were processed via solid-gas phase reactions using the hybrid precursor system chemical vapor deposition (HYSYCVD) route. SiCp porous preforms were infiltrated in subsequent stages (S1, S2) according to the following schedule: S1-1 and S1-2 at 1300 oC for 70 min in high purity nitrogen (HPN); S2 at 1350 oC for 120 min in ultra high purity nitrogen (UHPN). The composites were characterized by XRD, SEM and by means of He picnometry, volume-measurement approach and immersion in Hg using Archimedes's principle. Results show that atmosphere type and stage-processing approach affect the type, morphology and size of the nitrides formed. Stage-infiltration approach allows establishing conditions to control morphology, size (including nanometric size) and distribution of deposited phases, thus determining the properties of the composites.

9:50 AM
Transformation Plasticity in Rare Earth Orthophosphate/Orthovanadate Solid Solutions: Application to Fiber-Matrix Interphases in CMCs: *Randall Hay*[1]; Geoff Fair[1]; Emmanuel Boakye[2]; Pavel Mogilevsky[2]; Triplicane Parthasarathy[2]; [1]AFRL; [2]UES, Inc.

Oxide-oxide CMC's with rare-earth orthophosphate interphases such as monazite and xenotime have been successfully demonstrated. The major concern for these interphases is the high fiber pull-out stresses, typically ~80 - 200 MPa. An approach to lowering pullout stress involves use of interphases that weaken by transformation plasticity during a $-\Delta V$ martensitic phase transformation. The xenotime —> monazite martensitic phase transformation for rare-earth orthophosphate/orthovanadate solid-solutions was investigated for transformation plasticity during indentation. The ease of inducing the transformation and the subsequent effect of transformation plasticity on mechanical properties was assessed by the stress-strain behavior and hysteresis during indentation. The transformation extent and accompanying deformation were characterized by FIB and TEM of sections beneath the indents. Characterization was complicated by concerns about transformation of surface layers during polishing, and reversibility of the transformation with time. Processing methods necessary to deposit dense xenotime coatings near the xenotime-monazite phase boundary are discussed.

10:10 AM Break

10:30 AM

Creep and Fatigue Interactions of Haynes 282 at Elevated Temperatures: *Sara Longanbach*[1]; Carl Boehlert[1]; [1]Michigan State University

Superalloys can be considered as composite structures due to the significant strengthening offered by their precipitates. Haynes 282 is a wrought, gamma-prime strengthened nickel-based superalloy intended for use in high temperature structural applications. To investigate processing-microstructure-property relationships, the microstructure and elevated-temperature (760 – 815°C) creep and fatigue behavior were evaluated after processing involving strain-recrystallization treatments. Microstructural evaluation was performed using SEM and EBSD. General high angle boundaries (GHAB), low angle boundaries (LAB), and coincident site lattice boundaries (CSLB) made up 38%, 4% and 58%, respectively, of all the grain boundaries. It is noted that 47% of the boundaries were twins. The creep and fatigue properties of this alloy were compared to those obtained for two solid solution-strengthened superalloys, Haynes 230 and Udimet 188. The Haynes 282 alloy exhibited superior creep resistance. The deformation behavior and mechanisms will be discussed and particular emphasis will be placed on the grain boundary deformation.

10:50 AM

Oxidation of NixZry/Zr-4 Composite Surfaces: *Walter Luscher*[1]; Edgar Gilbert[1]; Stan Pitman[1]; [1]Pacific Northwest National Laboratory

Surfaces of Zircaloy-4 (Zr-4) components have been electroplated with nickel (Ni) and thermally treated to form a coherent, exterior layer of NixZry intermetallics. The result is a component with a graded composite surface consisting of discrete intermetallic layers over a Zr-4 substrate that exhibits two distinct stages of oxidation. Oxidation occurs rapidly at first as the intermetallic layer oxidizes, then slows asymptotically to a rate characteristic of the Zr-4 substrate as the intermetallic becomes saturated with oxides. This self-limiting oxidation behavior permits adequate structural integrity and mechanical strength of the substrate to be retained for the anticipated service environment. Microstructural evolution and elemental segregation determined by scanning electron microscopy and energy dispersive x-ray spectroscopy, respectively, correlates with isothermal weight gain data. An analysis of oxidation kinetics was also performed. Hardness and strength were evaluated via microindentation and tensile testing, respectively.

11:10 AM

Long Term Thermal Stability of Al_2O_3 Fiber (Sapphire) Reinforced NiAl Composites: *Jia Song*[1]; Weiping Hu[1]; Günter Gottstein[1]; [1]Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University

The long term thermal stability was tested for NiAl-Al_2O_3 composites. After the annealing of composites at 700°C and 1100°C for 2000 hours, the NiAl-Al_2O_3 system showed a good long term chemical stability. However, at such a high temperature, the grain growth and embrittlement took place in polycrystalline NiAl matrix. Besides, the corresponding interfacial shear strength was reduced from 222±50 MPa for the as-fabricated sample to 197±48 MPa and 150±38 MPa for the as-annealed samples at 700°C and 1100 C° respectively. Based on the microstructure changes and interfacial properties, the tensile strength was about 360 MPa for both as-fabricated and as-annealed samples at 700 °C, indicating a tiny change. But the tensile strength of the as-annealed samples at 1100 °C dropped to 170 MPa, 30 MPa lower than the value of 200MPa for the un-annealed one. The possible influences of microstructure and interface structure on mechanical properties are discussed.

11:30 AM

Synthesis and Deformation Behavior of Metal-Ceramic Nanolaminates: *Danny Singh*[1]; Nik Chawla[1]; Guanlin Tang[2]; Yu-Lin Shen[2]; Amit Misra[3]; Krishan Chawla[4]; [1]Arizona State University, School of Mechanical, Aerospace, Chemical, and Materials Engineering; [2]University of New Mexico/Department of Mechanical Engineering; [3]Los Alamos National Lab/CINT; [4]University of Alabama at Birmingham/Department of Materials Science and Engineering

Nanolayered composites are used in a variety of applications such as wear resistant coatings, thermal barrier coatings, optical and magnetic thin films, and biological coatings. Mechanical performance and reliability in all these applications is a key concern. In this talk we present a study of the synthesis, microstructural characterization, and deformation behavior of a nanolaminate metal-ceramic (Al/SiC) system. The nanolayered composite was processed by physical vapor deposition (PVD) using magnetron sputtering. Layer thickness and morphology were studied using a dual beam focused ion beam (FIB). Mechanical properties such as hardness and modulus were obtained using nanoindentation and micro-compression testing. Nanoscratch testing was conducted to quantify the resistance to wear and to estimate the adhesion strength between layers. Finally the damage mechanisms under various loading conditions were modeled using finite element modeling of the deformation process.

11:50 AM

Strengthening Behavior of Bilayer and Trilayer Cu-Based Nanocomposites: *Aikaterini Bellou*[1]; Nicole Overman[1]; David Bahr[1]; Hussein Zbib[1]; Ioannis Mastorakos[1]; Amit Misra[2]; [1]Washington State University; [2]Los Alamos National Laboratory

The effects of varying chemistry and individual layer thickness on the mechanical properties of Cu-based nanocomposites, of interest for a number of thin film applications, were investigated. Two different sets of samples were used. In the first case the thickness of the individual layers was kept constant at 20 nm while three different stacking sequences were used; Cu/Ni, Cu/Nb and Cu/Ni/Nb. Bulge testing and nanoindentation were utilized to evaluate the mechanical properties and especially the strength of the nanocomposites with the Cu/Nb system showing the higher hardness. The second set of multilayers involved only trilayer Cu/Ni/Nb films where the thickness of the Cu and Ni layers was maintained constant at 5nm while the thickness of the Nb layer ranged from 1 to 4 nm. The strengthening behavior of these films was again evaluated and comparison of the strengthening behavior of the Cu based multilayers with established models will be discussed.

Alternative Energy Resources for Metals and Materials Production Symposium: Session I

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division, TMS Light Metals Division, TMS: Energy Committee

Program Organizers: Ann Hagni, Geoscience Consultant; Neale Neelameggham, U.S. Magnesium, LLC; Aldo Steinfeld, ETH Zurich; Robert Palumbo, Valparaiso University

Wednesday AM — Room: 310
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Ann Hagni, Ann Hagni Consulting, LLC; Robert Palumbo, Valparaiso University

8:30 AM Introductory Comments

8:35 AM Keynote

The Global Scramble for Energy and Mineral Resources--Will the Move Towards Alternative Energy Sources Alleviate Our Import Problems?: *Vincent Matthews*[1]; [1]Colorado Geological Survey

Mineral and energy resources are being strained to supply increasing demand in established and emerging economies. Prices of natural-resource commodities dramatically escalated between 2003 and 2008 before plunging more steeply in four months, than in four years of the Great Depression. The competition to obtain a share of these natural resources became intense. The U.S. suffered from a shortage of several mineral commodities. From cement, to steel, to petroleum, to rare earth elements; the scramble for a piece of the worldwide pie is in a state the world has never known. The nation is being, and will be, significantly affected by this new world disorder. In addition to importing oil, natural gas, and uranium; the U.S. imports most of its needs for alternative energy technologies. China is taking advantage of the economic downturn to strengthen its position in mineral and energy commodities.

9:30 AM

Conceptual Process Plant Utility Schemes with Hybrid Energy System: *Neale Neelameggham*[1]; [1]US Magnesium LLC

Most of the chemical process plants and metallurgical production facilities already have some sort of co-generation to minimize process energy costs. Use of Alternative energy Production from sun and wind power with storage can become an integral part of a process plant utility. This will facilitate reduced fossil fuel usage, and help minimize thermal emissions. This will be similar to Pollution Control equipment which became essential parts of process plants in the past 4 decades. Conceptual flow sheets of such a Process utility schemes are presented.

9:50 AM
Advanced Electrochemical Storage R&D at PNNL for Renewable Integration and Utility Applications: *Zhenguo "Gary" Yang*[1]; Cheng Hung[1]; Daiwon Choi[1]; Gordon Graff[1]; Jianzhi Hu[1]; Soowan Kim[1]; Jun Liu[1]; Xiaochun Lu[1]; Kerry Meinhradt[1]; Vince Sprenkle[1]; John Lemmon[1]; Donghai Wang[1]; Guan-Guang Xia[1]; [1]Pacific Northwest National Laboratory

Growing world energy consumption, environmental concerns over the use of fossil fuels and the resource constrains have spurred great interests in renewable energy from wind and solar. To effectively use the renewable energy and to make it dispatchable, however, demand electrical energy storage (EES). EES is also a useful tool to improve reliability, stability and efficiency of future grids that is expected to be able to provide fuel (i.e. electricity) to plug-in hybrid vehicles. Among the most promising ones are electrochemical storage technologies or batteries that are capable of storing and releasing electrical energy in accordance with the demand. While a number of technologies have been developed or even demonstrated, there remain significant challenges in performance and cost for market penetration. As such PNNL has carried out wide research into advanced materials and EES technologies. This paper will report the efforts and discuss the needs, status and challenges.

10:10 AM Invited
Metal Ferrite Spinels for Solar-Thermal Water Splitting REDOX Cycles: *Alan Weimer*[1]; [1]University of Colorado

If H2 could be obtained cost effectively via the splitting of water using concentrated sunlight, then it's possible to operate a fuel cell using renewable H2 or to synthesize other fuels based on renewable H2 for generating electricity (H2 + CO2 ==> syngas ==> CH4) or for running internal combustion engines (syngas ==> methanol ==> gasoline). Spinel ferrites of the form MxFe3-xO4, where M generally represents Ni, Zn, Co, Mn, or other transition metals, have been shown to be capable of splitting water according to a two step REDOX solar thermochemical cycle. This presentation will focus on the thermodynamics and thermochemistry of solar-thermal chemical reaction processing with a special emphasis on the splitting of water using metal ferrites of the spinel structure. Experimental results for the REDOX reactions will be presented along with a possible process flow sheet (100,000 kg H2/day) and economic analysis (< $4/gge).

11:05 AM
Solar Thermal Electrolytic Production of Metals from Their Oxides: *Robert Palumbo*[1]; [1]Valparaiso University

Students and faculty at Valparaiso University launched a solar thermal electrolytic research program focused on the production of metals from their oxides. In this presentation, I describe the thermodynamic argument motivating the research and illustrate the influence of thermal transport processes such as electrolytic ionic conductivity and electrode reaction kinetics on the solar process. From this theoretical frame work, I present our experimental program and latest findings. Specifically, I show the ionic conductivities we established for mixtures of ZnO in Na3AlF6 and in xCaF2- y Na3AlF6 mixtures. I describe a 10 kW solar electrolytic reactor that we developed and are using to expose how ionic conductivity and electrode reaction kinetics influence process performance through operating variables and cell design variables. These influences are illustrated through interpretation of current vs. voltage maps as well as current vs. time plots for the electrolysis of ZnO within the temperature range of 1200-1500 K.

11:25 AM
CO2 Mitigation in Extractive Metallurgical Processes Using Concentrated Solar Energy: *Aldo Steinfeld*[1]; [1]ETH Zurich

Solar thermochemical processes make use of concentrated solar radiation as the energy source of high-temperature process heat. Considered are the thermal and carbothermal reduction of metal oxides for the production of metals, metal nitrides, and metal carbides. R&D work encompasses fundamental studies on thermodynamics, reaction kinetics, heat/mass transfer, and chemical reactor engineering. Solar reactor prototypes – at the 10 kW power level – are designed, fabricated, modeled, and tested in a high-flux solar furnace, further optimized for maximum solar-to-chemical energy conversion efficiency, and finally scaled-up for industrial applications – at the MW power level – using concentrating solar tower technology.

11:45 AM
Applications of Concentrating Solar Power in Materials Production: *Daniel Cook*[1]; Jordan Mayorga[1]; Joseph Kopp[1]; Robert Boehm[1]; [1]University of Nevada, Las Vegas

Solar generated power has long been considered a useful energy source only for low-energy density and non-mission critical use, such as providing electricity for residential applications. The success of Concentrating Solar Power (CSP) facilities, such as the 64 MW Nevada Solar-1 near Las Vegas, have demonstrated that solar does have application to high energy density industries such as materials and chemical production. This paper will discuss the current operating configuration of the Solar-1 facility and show how proposed modifications, such as addition of thermal storage and use of liquid salts as the working fluid, can further improve the efficiency and energy production of the plant.

12:05 PM
Radio-Thermionic Induced Reactions on Aluminum Based Materials and Their Correlation with Plasmon Formation and Tribocatalytic Mechanisms: *John Elton*[1]; James Cornwell[1]; [1]Protective Systems, Inc.

Thermionic induced reactions and radiation resonance catalysis of aluminum and aluminum oxide materials exposed to microwaves and triboemissions will be described and explained from both a fundamental and practical level. Magnetron operation at distinct operating conditions that generates both plasmon and triboemissive radiation will be explained and the resulting tribochemical and radiation resonance catalytic reactions between aluminum, aluminum oxide, water and graphite will be delineated. The generation of hydrogen from these materials using triboemissive radiation and microwaves will be described, and the application of this methodology for hydrogen based technologies will be discussed.

12:25 PM Concluding Comments

Alumina and Bauxite: Process Improvements and Experiences - Red Side II

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee, TMS: Aluminum Processing Committee
Program Organizers: Carlos Suarez, Hatch Associates Inc; Everett Phillips, Nalco Company

Wednesday AM Room: 611
February 17, 2010 Location: Washington State Convention Center

Session Chair: Shawn Kostelak, Gramercy Alumina

8:30 AM Introductory Comments

8:40 AM
Effect of Digesting Conditions on Physical Properties of Diaspore Red Mud: *Li Bao*[1]; Ting'an Zhang[1]; Zhihe Dou[1]; Guozhi Lv[1]; Xujian Wu[1]; Yongnan Guo[1]; Peiyuan Ni[1]; Jia Ma[1]; [1]Northeastern University

Diaspore, a kind of bauxite ore used to produce alumina, has complicated compositions and un-dense microstructure. The change of physical properties of diaspore is key to kinetic investigation of digesting process. Diaspore particles with the same particle size were digested under different digesting temperatures, times and stirring speeds. Specific surface area, pore volume and pore size of initial diaspore sample and red muds, the insoluble solid products during digesting process, were analyzed by nitrogen assorption-desorption measurement performed on ASAP 2020 Micromeritics apparatus. Meanwhile, Archimedes principle was employed to measure the densities of samples. The results show that digestion temperature and time bring about greater influence on the physical properties of particle samples than stirring speed.

9:10 AM
Extracting Alumina from Coal Flyash through Sodium Aluminate Solution in Soda-Sintering and Acid-Leaching Process: *Jilai Xue*[1]; Li Yan[1]; Yun Zhu[1]; [1]Unversity of Science and Technology Beijing

Coal fly-ash containing 40% -50%Al2O3 and 40-50% SiO2 from power plants is an alternative resource for alumina production. The alumina content in the coal fly-ash was extracted using soda-sintering and aluminate solution digesting process in laboratory. The sintering process was investigated using XRD, DTA and SEN-EDS techniques. The analysis showed that NaAlSiO4 was produced when the ratio of fly ash to Na2CO3 was 1:0.4 at 900°C, and the best leaching efficiency for the sintered NaAlSiO4 powders was obtained at the ratio 1:0.6. Removal of a glass-like silica layer on the surface of particles containing Al2O3/SiO2 in the fly ash. The so made sodium aluminate solutions after purification for removing Si and Fe were used to produce Al(OH)3 powders in a seeded precipitation process similar to Bayer's. This process can be an independent one or part of an ordinary industrial operation in alumina refining plants.

9:40 AM Break

10:00 AM
Improved Performance of Red Mud Settlers at Worsley Alumina: *Dane Eckart*[1]; John Kildea[2]; Peter Prinsloo[3]; David Nicholson[2]; Everett Phillips[4]; [1]Worsley Alumina Pty Ltd; [2]Nalco Australia Pty Ltd; [3]BHP Billiton; [4]Nalco Company

Efficient operation of the red mud removal system is a key operational goal for at Worsley Alumina. The plant has a series of high rate settlers employed as the primary solid/liquid separation step. Typically these vessels have used a combination of conventional polyacrylate flocculants and hydroximated polymers to deliver the required process targets. As part of a review of process efficiency Worsley has recently undertaken an assessment of Nalco's RRA polymer technology. Replacement of the conventional polyacrylate flocculant with a new RRA flocculant has led to substantial improvements in key process parameters for the vessels. Specifically use of the RRA polymer has resulted in significantly higher underflow solids density and more efficient overflow liquor filtration. Further optimization of the RRA technology has improved unit operation at a lower cost versus conventional product use. Use of the RRA technology is reviewed and further benefits from its use will be discussed.

10:30 AM
Redundancy of Security Filtration: *Peter-Hans ter Weer*[1]; [1]TWS Services and Advice

Security Filtration in the Bayer alumina refinery aims at controlling the contamination of alumina product by lowering the solids concentration in the decanter / settler overflow to the desired level in the Liquor to Precipitation (LTP). Significant strides have been made in the design of high rate thickeners and their feedwells, and similarly in the preparation of modern synthetic flocculants. Recent technological developments enable achieving solids levels in the bauxite residue settler overflow which are low enough to meet the targeted solids in LTP. This applies to existing refineries as well as to brownfield and greenfield projects.These developments provide an opportunity to lower alumina refinery operating and capital costs by (partly) by-passing or excluding the Security Filtration area. Savings include opex savings up to .8-1.5 $/tA and, in case of brownfield and greenfield projects, capex savings of 15-25 $/Annual tA.

11:00 AM
Tricalcium Aluminate Hexahydrate (TCA) Synthesis and Characterization: *Mamata Mohapatra*[1]; S. Acharya[1]; [1]Institute of Minerals and Materials Technology

Tricalcium aluminate hexahydrate (TCA) is an important filter-aid for Bayer's liquor (BL) polishing in addition to a few other applications. TCA can be prepared by reaction of CaO or $Ca(OH)_2$ in $NaAlO_4$ solutions preferably at low temperatures, [NaOH] and [CO_3^{2-}], however, various TCA sample properties influence efficiency of controlling the BL impurities. So the preparation of desired TCA samples under the synthetic conditions needs to be ascertained. In this study a synthesis approach for TCA was attempted using $Ca(OH)_2$ and $Al(OH)_3$ (gibbsite) at low temperature and [NaOH] under atmospheric pressure. To control the TCA synthesis process and the physicochemical properties further, a few simple surface active agents and ammonia-carbonate releasing reagents are tested. The effect of temperature, particle dispersion, NaOH and time on particle size and morphology, reactant surface coating and TCA product phase formation were analyzed using various analytical techniques. This kinetic study provides some insight into the TCA formation mechanism and interaction of various synthesis parameters influencing the TCA physicochemical properties.

11:30 AM
Effect of Carbide Slag on High Pressure Digestion Properties of Diaspore: *Wang Bo*[1]; Sun Huilan[1]; Bi Shiwen[2]; [1]Hebei University of Science and Technology; [2]Northeastern University

Carbide slag is one of the industrial waste residue in the production of acetylene, and it pollutes the environment seriously. Carbide slag was used to replace lime as the additive during high pressure digestion of diaspore in this paper. The effect of carbide slag on the digestion and settling properties of diaspore was studied, and the mechanism of carbide slag during the high pressure digestion process was also investigated by XRD, SEM and EDS methods. The results indicated that the alumina relative digestion rate of diaspore could reach 96% when the addition of carbide was 18%. If the additive was lime, its addition was 10% during this digestion rate. The existence of carbide slag could improve the settling properties of the slurry after alumina digestion compared to the addition of lime. The action mechanism indicated that carbide slag could accelerat the formation of sodium-silicon residue during high pressure digestion process.

Aluminum Alloys: Fabrication, Characterization and Applications: Fatigue and Corrosion

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Processing Committee
Program Organizers: Subodh Das, Phinix LLC; Steven Long, Kaiser Aluminum Corporation; Tongguang Zhai, University of Kentucky

Wednesday AM — Room: 615
February 17, 2010 — Location: Washington State Convention Center

Session Chair: Tongguang Zhai, University of Kentucky

8:30 AM
Corrosion-Fatigue Interactions in Hollow AA6XXX Alloy Extrusions: *Nicholas Nanninga*[1]; Calvin White[2]; [1]NIST; [2]Michigan Technological University

The effect of an aqueous 3.5 wt% NaCl environment on the high cycle fatigue properties of hollow AA6082 and AA6063 extrusions has been evaluated. These two alloys have contrasting extrusion microstructures, with the AA6063 alloy being fully recrystallized, and the AA6082 alloy retaining a fully fibrous core microstructure with a recrystallized surface layer. Both alloys exhibited substantial reductions in their fatigue lives when exposed to the salt solution. The environmental effect on fatigue appears to be primarily associated with pitting and intergranular corrosion, which leads to premature fatigue crack initiation. Fatigue properties were most severely affected at low stress amplitudes (longer fatigue lives), probably as a result of the more extensive pitting and intergranular corrosion that occurred in those specimens.

8:50 AM
Corrosion Fatigue and Stress-Corrosion Crack Growth in Sensitized Al 5083: *Peter Pao*[1]; Ramasis Goswami[2]; Ronald Holtz[1]; [1]Naval Research Laboratory; [2]SAIC

The corrosion fatigue and stress-corrosion crack growth kinetics of sensitized (175 °C/10 days) and as-received (H131) Al 5083 were investigated. TEM investigations reveal the presence of continuous magnesium-rich ß phase (Al3Mg2) at the grain boundaries in sensitized Al 5083 while in as-received Al 5083-H131 such ß phase is absent. The saltwater stress-corrosion cracking threshold of sensitized Al 5083 is significantly lower than that of the as-received Al 5083-H131. While the saltwater corrosion fatigue cracking thresholds of sensitized and as-received Al 5083 are comparable at a low stress ratio, the corrosion fatigue threshold is significantly lower and crack growth rate significantly higher in sensitized Al 5083 than those of as-received Al 5083. The observed fatigue crack growth and stress-corrosion cracking responses are discussed in terms of differences in microstructure and the interplay between stress-corrosion and corrosion fatigue cracking thresholds.

9:10 AM
Environmental Degradation of SCC-Affected Fatigue Life of High-Strength Aluminum Alloys and Prediction Methodology for Remaining Fatigue Life in Aging Aircraft: *Yooin Jeong*[1]; Hyunjung Lee[2]; Eungyeong Lee[2]; Haksu Kim[2]; Cheolju Lee[1]; Sangshik Kim[2]; [1]Korea Aerospace Industries, LTD.; [2]Gyeongsang National University

There is a need to understand the effects of environmental degradation on fatigue and stress corrosion cracking (SCC) behaviors for predicting the remaining life of aging aircraft. In this study, hour-glass type specimens were prepared from aging aircrafts, the parts of which had been in service and stored after retirement, and S-N fatigue tests were conducted and the results were compared to those of pristine specimens. Smooth bar and single edge notch specimens were also prepared, and slow strain rate tests were performed to determine the effect of SCC. The present study demonstrates that the environmental degradation, predominantly corrosion pits, significantly reduces the fatigue life, and the SCC contribution needs to be considered for accurate remaining fatigue life prediction. Based on the fracture mechanics-based SCC data and the actual fatigue data, several prediction methodologies for remaining fatigue life are discussed with quantification of corrosion and modeling of crack propagation.

9:30 AM
Effect of Heat Treatment on Corrosion Behavior of Aluminum-Lithium Alloy 8090: *Amr Kobeisy*[1]; Ahmed Metwali Abd El-Aziz[1]; Randa Abdel-Karim[2]; Abdel-Aziz Waheed[3]; [1]German University in Cairo; [2]Cairo University; [3]Atomic Energy Authority

Al-Li 8090 alloy was subjected to different retrogression and reaging (RRA) treatments to investigate their effects on the mechanical and corrosion properties in comparison to peak aged (PA) condition. Optical microscopy, scanning electron microscopy, x-ray diffraction, hardness and tensile measurements were used. Stress corrosion cracking and salt spray tests were carried out and results were compared with microstructure and mechanical properties.The RRA 170 and 190 treatments' corrosion resistance have deteriorated in both tests compared to the PA, while the RRA 210 treatment showed the same atmospheric corrosion resistance as PA. However, RRA 210 showed a much lower SCC resistance, even lower than the RRA 170 and 190 treatments. The results have been explained by the anodic dissolution of uneven distributed phases on the grain boundaries. These precipitations created micro-galvanic cells and thus accelerating localized anodic dissolution mechanism. Pitting and intergranular stress corrosion cracking were found to be the corrosion mechanisms.

9:50 AM
Multi-Axial Fatigue Behaviour of A356-T6: *Matthew Roy*[1]; Yves Nadot[2]; Daan Maijer[1]; [1]The University of British Columbia; [2]Ecole Nationale Supérieure de Méchanique et d'Aérotechnique (ENSMA)

As light castings become commonplace in transportation applications, design tools must capture multi-axial fatigue effects for structural components. In this investigation, uni-axial and multi-axial fatigue tests have been conducted to investigate the fatigue behaviour of A356-T6 casting alloy in the high cycle regime. The step technique was used to determine the fatigue limit at a million cycles for material with different microstructure. Through tension and torsion testing of specimens with artificial defects, the fatigue mechanism is scrutinized and the crack growth rate has been tabulated for using the replica technique. These results are used to discuss the suitability of treating defects as cracks using linear fracture mechanics. For different loading cases, the stress distribution around defects is examined to understand the role of the stress state in the fatigue process. The results are applied to other classical multi-axial fatigue criterion (Crossland and Van Dang), and one based on principal stresses.

10:10 AM
Processing of Ultra-Fine Grain Structure in Aluminium Alloy by Equal Channel Angular Pressing: Narasimhan Narayani[1]; Prasad Shanmugasandaram[1]; C. K. Gopalakrishnan[1]; R. Hariharan[1]; G. Swarupini[1]; *S. Balasivananda Prabhu*[1]; [1]Anna University

The paper involves developing nanostructured Al6061 particles,characterizing their unique mechanical properties and microstructure. Equal Channel Angular Pressing (ECAP), a discontinuous process for Severe Plastic Deformation (SPD) is used. The Ultra Fine Grain microstructure of the material is characterized by TEM, SEM and XRD to identify their high angle strain, low angle strain and other strength related properties. A split die of required dimensions to produce maximum possible strain without causing failure is used for the process. The resulting Aluminium 6061 alloy material can be widely used in aerospace industries where the proposed increase in density and toughness will make a very big impact. Sports, yatch construction, automotive industries also stand to gain out of this project. The characterization will give researchers and industrialists better insight into the mechanical behaviour and properties of Al 6061 processed through ECAP. Suggestions relating to more optimized die design and lubrication aims at making ECAP a more efficient and effective production process for bulk materials.

10:30 AM Break

10:45 AM
Fatigue in Friction Stir Welded 7050 Al: *Ashley Teare*[1]; Adam Hein[1]; Aaron Wilkinson[1]; David Field[1]; Tracy Nelson[2]; [1]Washington State University; [2]BYU

The fatigue life of a friction stir welded 7050 aluminum alloy was investigated. Measurements of grain boundary structure and local texture were made by electron backscatter diffraction to investigate the correlation between local structure and fatigue life. Miniature single edge notch fatigue specimens were machined from various regions of the weld nugget and surrounding thermo-mechanically and heat affected material. These were tested to obtain fatigue life data for local regions in the welded plate. A strong gradient of fatigue behavior was observed with fatigue life being maximized in the weld nugget center and increasingly shorter life for specimens near the advancing and retreating edges of the weld and into the heat affected regions. Local microstructure was observed to play a significant role in fatigue life performance.

11:05 AM
Effects of Multipass Friction Stir Processing on Microstructure and Mechanical Properties of Al-Zn-Mg (7039) Alloy: *Prashant Soni*[1]; Bhagwati Kashyap[1]; N. Prabhu[1]; A.G. Rao[1]; V. Deshmukh[1]; [1]IIT Bombay

Hot rolled Aluminum 7039 sheets were subjected to Friction Stir Processing (FSP) up to three passes for grain refinement. The grain size was found to decrease from the initial value of 50 µm to 10 µm after two passes in the nugget zone. The number of FSP pass was continued to explore further evolution in microstructure. Precipitate size and distribution were investigated in the nugget zone, thermo-mechanically affected zone and heat affected zone as a function of number of passes and the same were related to its role in the mechanism for grain growth in quasi-single phase system. Tensile tests were conducted at room temperature and elevated temperatures. Hall-Petch type relation was obtained at low temperature whereas the fine equiaxed microstructure of grain size less than 10 µm exhibits superplastic behavior.

11:25 AM
Influences of Tool Pin Profile and Welding Speed on the Formation of Friction Stir Welding of AA7075 and AA5083: *Reza Behnagh*[1]; Mohammad Kazem Besharati[2]; [1]Tehran University; [2]Department of Mechanical Engineering, Tehran University

Friction stir welding (FSW) process is an emerging solid state joining process in which the material that is being welded does not melt and recast. This process uses a non-consumable tool to generate frictional heat in the abutting surfaces. The welding parameters and tool pin profile play major roles in deciding the weld quality. In this investigation, an attempt has been made to understand the effect of welding speed and tool pin profile on friction stir welding formation of AA7075 and AA5083. Tow different tool pin profiles (cylindrical,tapered cylindrical) have been used to fabricate the joints at different weding transverse and rotational speeds. It is found that the threaded tapered cylindrical tool produces mechanically sound and metallurgically defect free welds compared to other tool pin profile.

11:45 AM
Tensile Properties of a Friction Stir Processed Al-Cu 2218 Alloy at Elevated Temperatures and Related Microstructural Characteristics: *Ssu-Ta Chen*[1]; Truan-Sheng Lui[1]; Li-Hui Chen[1]; [1]Department of Material Science and Engineering, National Cheng Kung University

Tensile properties of extruded Al-Cu 2218 base metal and friction stir processed (FSPed) Al-Cu 2218 specimens at elevated temperatures are carried out in this study. From room temperature to 300°, FSPed specimens exhibit higher tensile yield stress than base metal. The higher yield stress of FSPed specimens is resulted mainly from natural aging and minor from grain-refinement. The advantage of FSPed sample disappears and simultaneously accompanies by an increasing total elongation when tensile tests are conducted at 400° and 450°, respectively. To compare with base metal, FSPed specimens have a more pronounced increasing in total elongation. The excellent total elongation of FSPed specimens is a consequence of dynamic recrystallization and grain boundary sliding.

12:05 PM
Effect of Porosity on the High-Cycle Fatigue Properties of 356 Casting Aluminum Alloy: Young-Jae Lee[1]; Kwang-Jun Euh[2]; Kyu-Sang Cho[3]; *Kee-Ahn Lee*[4]; [1]Center for Advanced Green Materials Technology, Andong National University; [2]Korea Institute of Material Science; [3]Dongyang University; [4]Andong National University

The effect of porosity on the high-cycle fatigue properties of A356 casting aluminum alloys was investigated in this study. The high-cycle fatigue results indicated that the fatigue strength of the 356-T6 (heat-treated) alloy was higher than that of the 356-F (casted) alloys because of the significant reduction in volume fraction of pores by heat treatment. The SEM fractography results showed that porosity affected detrimental effect on the fatigue life: 80% of all tested samples fractured as a result of porosity which acted as the main crack initiation site. It was found that fatigue life decreased as the size of the surface pore increased. A comparison was made between surface pore and inner pore for its effect on the fatigue behavior. The results also showed that the fatigue strength with the inner pores was higher than that of the surface pore. *This research was supported by Materials Bank Program, Korea.

Aluminum Reduction Technology: Hall-Héroult Cell: Processes Modeling and Aluminium Smelter Modeling

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee, TMS: Aluminum Processing Committee
Program Organizers: Charles Mark Read, Bechtel Corporation; Gilles Dufour, Aluminerie de Deschambault

Wednesday AM — Room: 608
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Marc Dupuis, GéniSim Inc; Daniel Richard, Hatch

8:30 AM Introductory Comments

8:40 AM
Mathematical Modeling of Aluminum Reduction Cell Potshell Deformation: *Marc Dupuis*[1]; [1]GéniSim Inc

One of the key component of an aluminum reduction cell design is the potshell design. The potshell must be designed in such a way that it will not deform excessively in operation and will remain as much as possible in elastic deformation mode. Yet, heavy over-designed potshells are very costly hence the importance of producing a close to optimal design where all structural elements are getting their fair share of the total load while being charged close to their elastic limit.Producing such an optimal potshell design would be very time consuming without the extensive usage of modeling tools. Three such tools are presented here in order of complexity, namely: the empty shell, the almost empty shell and the half empty shell ANSYS® based thermo-mechanical models. Results are presented for each model solved both in elastic and plastic modes as well as the CPU time required to solve them.

9:10 AM
The Use of CFD Simulations to Optimise Ventilation of Potrooms: *André Maarschalkerwaard*[1]; [1]Colt Technology

Ventilation in potrooms has always been a hot issue. Well engineered systems to evacuate the surplus of thermal energy from the potrooms are mandatory, and should be given the attention that they deserve. Insufficient ventilation could lead to overheating of pots with the accompanying problems. Simulations can help in optimising the ventilation and gives better understanding of the behaviour of airflows inside the building. Besides the main focus on productivity, attention should be given to the exposure of operators to HF concentration and high temperatures. A well designed ventilation scheme can help to create a healthy and safe environment for the operators.Airflows outside the building can be investigated with the same simulation technique, providing information about the spreading of contaminated airflows.

9:40 AM
Safe and Efficient Traffic Flow for Aluminum Smelters: *Laszlo Tikasz*[1]; Charles Read[1]; Robert Baxter[1]; Rafael Pires[1]; Robert McCulloch[1]; [1]Bechtel

Aluminum smelter design, construction and operation requires: in-depth knowledge of smelter operations; integration of engineering disciplines; process modeling and dynamic simulation expertise. This paper outlines an approach for improving plant configurations by applying Safety by Design and Lean Manufacturing Methods to achieve a safe and efficient plant design that delivers value over the entire life cycle of the plant, from early project definition, through execution and beyond operational start-up. Design steps used to develop the improved layout include activities such as: listing and specifying movements of People, Products and Materials between Customer and Supplier connections, identifying and quantifying traffic-related hazards, developing and comparing alternative solutions that offer a safe and efficient road network, and traffic scheduling for vehicles and pedestrians throughout the Smelter. To demonstrate the method applied, examples from a Plant Traffic Model and comments on typical traffic risks are presented.

10:10 AM
Development and Application of an ANSYS® Based Thermo-Electro-Mechanical Anode Stub Hole Design Tool: *Marc Dupuis*[1]; [1]GéniSim Inc

At the 2009 TMS conference, we could observe a renewed interest for the optimization of anode stub hole design. This is not surprising considering that we can estimate that the contact resistance voltage drop at the cast iron/anode carbon interface is about 60 mV (assuming 0.1 m2 of contact surface per stub hole, 3000 A of current per stub and 2 micro-ohm m2 of the average contact resistance) which translate to 1.2 MM$ per year of operational cost for a typical modern smelter for that contact resistance alone.Hence, it is easy to understand that there is a good incentive to optimize the stub hole design in order to minimize the cast iron/anode carbon contact resistance voltage drop. For that purpose, the author took advantage of the recent development of ANSYS® contact elements library to develop an ANSYS® version 12.0 based fully coupled TEM anode stub hole design tool.

10:40 AM Break

10:50 AM
Effects of High Temperatures and Pressures on Cathode and Anode Interfaces in a Hall-Heroult Electrolytic Cell: *Lyne St-Georges*[1]; [1]UQAC

This paper deals with the physical modifications occurring at high temperatures and pressures at the interfaces found in the anode and cathode of a Hall-Heroult electrolytic cell. The anode and the cathode are fabricated with carbon blocks, were steel bars are inserted and sealed with cast iron. Consequently, their interfaces are composed of cast-iron and steel and of cast-iron and carbon. For the investigation presented here, an experimental setup was build to heat and load anodic and cathodic samples. A specific attention was put on the samples preparation, to reproduce real cathode/anode sealing conditions. During the heating and the loading of the samples, fluctuations of electrical and thermal contact resistances are observed and related to physical transformation at the interfaces. These transformations could explain the fluctuations of electrical and thermal contact resistances observed and potentially the non-homogeneities of voltage and current distribution occurring in a Hall-Heroult electrolytic cell.

11:20 AM
Design of a Bypass Joint for the Aluminum Reduction Cells.: Yimy Sarkis[1]; [1]Morochos JJ C.A.

This paper presents the design of an electrical joint for the by-pass system of 230kA cells of Aluminum Reduction that produce lower values of voltage drop and enhanced ergonomics for the installation, using a FEM code with interface contact elements, thermo-electrical and thermo-mechanical non-linear simulations were conducted, using properties such as thermal expansion and electrical and thermal contact resistance determined by mathematical models that depends on surface roughness and pressure, the first analysis was the study of the current joint's behavior, which determined that contact occurs only at discrete parts of the interface, then the proposed design model that has a system for pressure adjustment to increase contact pressure and distribute it evenly, making better use of the contact area, therefore, the electrical and thermal contact conductance increase, which is reflected in a decrease of temperature values up to 20,47% and voltage drop up to 36,5%, generating substantial energy savings.

11:50 AM
3D Freeze Shape Study of the Aluminum Electrolysis Cells Using Finite Element Method: Cui Xifeng[1]; Zhang Hongliang[1]; Zou Zhong[1]; Li Jie[1]; Lai Yanqing[1]; Xu Yujie[1]; Zhang Hehui[1]; *Lv Xiaojun*[1]; [1]Central South University

A proper shape of the frozen electrolyte on the sidewall is vital for the aluminum reduction cells. Its formation is influenced by sorts of factors. In this paper, the impact of some parameters upon the shape of the side-ledge is assessed based upon a quarter 3-D thermal-electric ANSYS finite element model, which is developed to fulfill the 3-D calculation of side-ledge. The model has been validated using measurements from a 300kA cell. The influence of the parameters, such as the ACD, the anode change, the anode-channel width, the heat preservation situation of the bottom, side and top, and the property of the cathode block are discussed. Various recommendations are correspondingly made to obtain a proper frozen electrolyte layer.

12:20 PM Concluding Comments

Aluminum Reduction Technology: Hall-Héroult Cell: Processes Modeling and Measurements

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee, TMS: Aluminum Processing Committee
Program Organizers: Charles Mark Read, Bechtel Corporation; Gilles Dufour, Aluminerie de Deschambault

Wednesday AM Room: 614
February 17, 2010 Location: Washington State Convention Center

Session Chairs: Nobuo Urata, Alumilab; James Evans, University of California, Berkeley

8:30 AM Introductory Comments

8:35 AM
CFD Modelling of Effect of ACD and Anode Size on Alumina Mixing in Aluminium Reduction Cells: Yuqing Feng[1]; *Mark Cooksey*[1]; Phil Schwarz[1]; [1]CSIRO Minerals

Aluminium reduction cells have been continuously improved to reduce energy consumption and increase metal production rates , eg by reducing anode-cathode distances (ACDs). Line currents have been increased to increase production rates, which often requires larger anodes to maintain an acceptable current density. These changes may have a significant impact on aspects of cell performance such as bath flow and alumina mixing. In previous work, a computational fluid dynamics (CFD) model of bath hydrodynamics in aluminium reduction cell has been developed and validated using water model data and plant measurement. In the present work, the validated CFD model has been extended to study the effect of ACD and anode size on bath flow and alumina mixing in a typical full-scale industrial cell. The relative effect of ACD and anode size has been compared in terms of bath flow, gas layer thickness in the ACD, and alumina mixing kinetics.

9:00 AM
Terminating Anode Effects by Lowering and Raising the Anodes - A Closer Look at the Mechanism: *Jomar Thonstad*[1]; Helmut Vogt[2]; [1]Norwegian University Sc. Technology; [2]TFH, University of Applied Sciences

In aluminium cells anode effects are unwanted events, leading to a waste of energy, overheating and emissions of PFC gases that have a high environmental impact. A common way to quench anode effects in prebake cells is to lower and raise the anodes repeatedly, so-called “anode pumping”. This method is normally very effective, the anode effect going off when the anodes are in the low position. The actual mechanism has been the subject of some controversy, explanations varying from: (1) the effect of exposing fresh anode surface area, (2) lowering the anode current density by exposing a larger active anode surface area, or (3) making short circuits to the metal pad. Based on a mathematical model the present work discusses the mechanism, focussing on the enhancement of the anode surface area.

9:25 AM
Bath Temperature Inference through Soft Sensors Using Neural Networks: *Fabio Soares*[1]; Roberto Limao[2]; Marcos Castro[3]; [1]Exodus; [2]UFPA; [3]Albras

The thermal balance has a direct impact in current efficiency, however its measures are subjected to hardware and human errors, and normally it takes a long time between measures in the same cell. Those kind of process variables have lately been estimated with the aid of soft sensors, which are computational intelligence algorithms used for complex processes modeling. Since they are software based, they are not subjected to hardware failures and can estimate any process variable according to the data history and available plant operation knowledge. With soft sensors, online temperature estimation is possible, allowing plant operators to early detect process abnormalities and plot trends without needing to perform a real measure. A case of a soft sensor for online temperature estimation in an important brazilian aluminium smelter is presented in this work, since its design through implementation at production, according to a research methodology.

9:50 AM
The Determination of Pot Current Distribution by Measuring Magnetic Fields: Nobuo Urata[1]; *James Evans*[2]; [1]Alumilab; [2]UC, Berkeley

A couple of previous papers have suggested that the current distribution in a pot can be determined by measuring magnetic fields, e.g. the distribution of current among the anode rods can be found by placing a magnetic field sensor next to each rod. Because the current distribution can have a significant effect on pot performance, the suggestion is worth analyzing and this has been done by mathematical models in the present paper. One important aspect of such measurements is the effect of fields generated by other currents on the measurement of a particular current, e.g. the effect of currents in adjacent anode rods on the measurement for one rod. It is shown that, with the use of a sufficient number of sensors, it should be possible to de-convolute individual anode currents, and other currents, from the measured field values.

10:15 AM Break

10:25 AM
Busbar Circuit Design and Installation for Boosting Already Boosted Pots: Daniel Champagne[1]; Donald Ziegler[2]; Andre Schneider[1]; *Daniel Richard*[1]; [1]Hatch; [2]Alcoa

This tight-schedule project was an important milestone in the announced modernization of the Baie-Comeau Smelter plant. In the spring of 2008, an integrated Alcoa-Hatch multidisciplinary team succeeded to install in record time a new booster rectifier circuit for testing prototype pots. A unique feature of this project is that the new circuit is boosting already boosted pots. To emulate the magnetic field that would affect the pots once the whole potline operates at the target amperage, the new circuit includes a split booster input circuit. Also, in order to accommodate changing conditions in the line and two boost rectifiers, a custom-designed variable electrical resistance was also installed to control the current split in the booster input branches. By using available equipment, a very tight timeline was achieved, and the new systems were put in place with the potline running and with no loss-time injury.

10:50 AM
Study of Surface Oscillation of Liquid Aluminum in 168kA Aluminum Reduction Cells with a New Type of Cathode Design: Wang Ziqian[1]; *Feng Naixiang*[1]; Peng Jianping[1]; Wang Yaowu[1]; Qi Xiquan[2]; [1]Northeastern University; [2]Northeastern University Engineering & Research Institute Co. Ltd.

The surface oscillation of liquid aluminum in the new type of cathode structure in 168kA aluminum reduction cells was measured by a dynamic detecting system of surface oscillation of liquid aluminum which is designed independently to research the mechanism on energy saving. The measurements show that the cathode convex in the new type of cathode could reduce the velocity of liquid aluminum and could weaken the surface oscillation of liquid aluminum, so the energy consumption could be reduced by decreasing interpolar distance. The surface oscillation of liquid aluminum was not be affected by the operation of metal tapping but it was affected greatly by anode changing. After anode changing, the periodic time is changed a little. Typically, the periodic time of liquid aluminum wave in the new type of cathode aluminum reduction cells is 50 s, the average velocity of the liquid aluminum wave is 0.12 m/s, and the wavelength is 6 m.

11:15 AM
Modelling and Optimization of Busbar Configuration in Aluminum Electrolysis Cell with Genetic Algorithm: *Mao Li*[1]; [1]Central South University

Based on the commercial package ANSYS and custom APDL code, a parametrical mathematic model of busbar configuration in aluminum electrolysis cell was proposed. An object function was established based on a simplified magnetohydrodynamic stability criteria, the parameters of busbar configuration model was studied and optimized automatically with genetic algorithm according to the value of custom object function. It is shown that the parametrical busbar configuration model can be established and calculated adaptively to find the optimal busbar configuration, the physical fields of the cell after busbar optimization is also discussed, cell with optimized busbar configuration has shown satisfying distribution of physical fields.

11:40 AM Concluding Comments

Biological Materials Science: Mechanical Behavior of Biological Materials III: Soft Tissues and Materials

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS: Biomaterials Committee, TMS/ASM: Mechanical Behavior of Materials Committee
Program Organizers: John Nychka, University of Alberta; Jamie Kruzic, Oregon State University; Mehmet Sarikaya, University of Washington; Amit Bandyopadhyay, Washington State University

Wednesday AM February 17, 2010
Room: 205
Location: Washington State Convention Center

Session Chairs: Po-Yu Chen, University of California, San Diego; Roger Narayan, NC State/UNC Chapel Hill

8:30 AM Invited
Using Optical Tweezers to Probe Mechanical Response from Single Molecules to Soft Biological Materials: *Nancy Forde*[1]; [1]Simon Fraser University

In the past decade, the ability to manipulate and measure forces exerted by single biological molecules has transformed our understanding of their mechanical response, stability, and the mechanisms by which they operate. One of the essential tools in this revolution has been optical tweezers, which use a focused laser beam to "trap" (hold stably in three dimensions) micrometer-sized refractive particles. In this talk, I will briefly describe how optical tweezers work and how they can be used to manipulate and probe the mechanical response of single protein molecules. I will then discuss our work developing the technique of holographic optical tweezers as a microscale tensometer for soft materials, capable of straining and measuring stresses on materials in three dimensions. We are applying these techniques to learn about the molecular basis for mechanical response of the extracellular matrix proteins collagen and elastin.

9:00 AM Invited
Investigating the Structure-Properties Relationship of the Cornea and Sclera: Brad Boyce[1]; Thao Nguyen[2]; [1]Sandia National Laboratories; [2]Johns Hopkins University

We are developing an integrated experimental and modeling program to investigate the relationship between the structure, mechanical behavior, and physiologic function of the cornea and sclera. Central to the program is an inflation testing method that uses digital image correlation (DIC) to provide a three-dimensional deformation map of the exposed surface of the specimen. We have developed the method for bovine, human, and mouse tissues. Human and mouse experiments compare the anisotropic viscoelastic behavior of tissues of normal and clinically diagnosed glaucoma (human) and induced glaucoma (mouse) eyes. Inflation experiments do not measure directly the stress response of the tissues and require a constitutive and finite element modeling to process the results. For glaucoma, we also apply the models to probe the effects of the measured differences in the properties of the cornea and sclera on the deformation and stress state of the optic nerves.

9:30 AM Invited
Polymer Mechanics Models the Fraction of Cartilage Stress Relaxation Not Caused by Fluid Flow: *David Fyhrie*[1]; R. June[2]; Corey Neu[3]; Justin Barone[4]; [1]University of California, Davis; [2]University of California, San Diego School of Medicine; [3]Purdue University; [4]Virginia Technological University

Stress relaxation of calf cartilage for less than ≈1 sec is best modeled using a monodisperse polymer model but for ≥1 sec (up to 1800 seconds) a combination of elastic response, inviscid fluid flow (KLM model) and a polymer fluid accurately fits the experimental data. Relaxation of polymer fluids is often approximated by the Kolrausch-Williams-Watt (KWW or stretched exponential) function. We derive a new application of the KWW function based on random bonding of linear macromolecules. Analysis of the experimental data demonstrates a transition between relaxation dominated by fluid flow and relaxation dominated by polymer mechanics. The best fit to the experimental data was consistent with our analysis of the random bonding mechanism. The conclusion is that stress relaxation in calf cartilage is well approximated by a KWW function with a shape exponent consistent with the mechanism of relaxation dispersion being random bonding between linear polymers.

10:00 AM
Stimulated Cellular Response of Novel Hybrid Bimodal Network Elastomers for Soft Tissue Implants: *Wah Wah Thein-Han*[1]; Jinesh Shah[1]; Devesh Misra[1]; [1]University of Louisiana

In reconstructive surgery, tissue transplantation and/or tissue substitute transplantation approaches are widely used to reconstruct and repair the deformity and defects of human organs. In this regard, we describe here the synthesis and biological property of novel hybrid bimodal network elastomers that are characterized by high strength-high ductility combination and good biocompatibility. Pre-osteoblasts grown on hybrid network were well spread, flat, large in size with rough cell surface, and appeared as a group. In contrast, these features were less pronounced in pure elastomers (e.g. smooth cell surface, not well-spread). Interestingly, immunofluorescence study illustrated distinct fibronectin expression level, stronger vinculin focal adhesion contacts associated with abundant actin stress fibers in pre-osteoblasts grown on the composite compared to silicone rubber, implying enhanced cell-substrate interaction.

10:20 AM Break

10:30 AM Keynote
Nanomechanical Properties of Biological Tissues – Pushing the Boundaries of Nanoindentation Testing: *Michelle Dickinson*[1]; [1]Auckland University

Biological tissues consist of a complex hierarchical architecture at a range of length scales from nano to macro. Each of these components combine to perform diverse mechanical, biological and chemical functions which are ever-changing. Many diseases are not diagnosed until catastrophic failure occurs, such as a broken bone or tendon rupture. However, these may have been preceded by significant microstructural changes which, if detected early can lead to identification of the key contributing failure mechanisms. Nanoindentation testing on these biological materials is becoming more popular. This paper highlights recent work measuring individual components within biological tissues including single osteons in bone, collagen fibrils in vertebrae and calcified deposits on smooth muscle walls. The results show how testing structures at the nanoscale can relate each component to the micro, and bulk properties. By studying healthy and diseased tissues at the nanoscale, a more targeted approach to disease progression/prevention can be pursued.

11:10 AM
Dynamic Nanoindentation of Articular Cartilage: Oliver Franke[1]; Mathias Göken[2]; Marc Meyers[3]; Karsten Durst[2]; *Andrea Hodge*[4]; [1]MIT; [2]University of Erlangen; [3]University of California, San Diego; [4]University of Southern California

A technique to study the time-dependant properties of hyaline porcine cartilage under in vitro conditions is presented. The tests were carried out in a wide range of frequencies from 1 Hz to 250 Hz on frozen and fresh samples. While the fresh samples show storage moduli between 3.6 MPa and 8 MPa (for 1 Hz to 20 Hz), freezing lowers the values for the surface region by a factor of 2. The same trend was observed for the loss modulus. Since the classical contact area determination for sharp indenters in viscoelastic materials is expected to be inaccurate a new method is introduced using the same approach used for the pile-up corrected hardness. An internal calibration on the tested material is required as the values may vary from spot to spot or between samples. It will be shown, how this can be achieved using different loading profiles and frequencies.

11:30 AM
Nanoindentation of Ultrasoft Biological Materials: *Vinod Nayar*[1]; Andrea Hodge[2]; James Weiland[3]; [1]University of Southern California - Department of Biomedical Engineering; [2]University of Southern California - Department of Aerospace & Mechanical Engineering; [3]University of Southern California - Keck School of Medicine

The methodology and analysis for testing sclera tissue by nanoindentation are presented. Using a Hysitron Triboscope nanoindenter, a reduced modulus of 31.50 ± 8.30kPa and hardness of 0.19 ± 0.09kPa were obtained from harvested porcine, posterior-sectioned, sclera in room temperature saline conditions with a load-controlled, flat punch, fluid-cell, sapphire tip. This methodology has significantly improved upon the consistency of previous studies and will allow for further studies of similar ultrasoft biological materials. Previous nanoindentation studies have focused on both hard and soft biological materials, ranging from dentin and cortical bone to arteries and cartilage. In contrast, the sclera tissue is considered an ultrasoft material since it has a reduced modulus less than 1MPa. The effect of factors including drift monitoring, hydration conditions, spring force corrections, mounting procedures, peak loads, and selection of load functions are also discussed.

11:50 AM
Quantitative Viscoelasticity Measurements of Biological Materials by Atomic Force Acoustic Microscopy: *Arnaud Caron*[1]; Ansgar Hohmann[2]; Erhard Stupperich[3]; Franz-Günter Sander[2]; Hans-Jörg Fecht[1]; [1]Institute of Micro- and Nanomaterials, University Ulm; [2]Department of Orthodentics, University Ulm; [3]Institute of Microbiology and Biotechnology, University Ulm

Atomic Force Acoustic Microscopy (AFAM) is a resonance spectroscopy technique where a micro-fabricated cantilever beam in contact with a sample surface is excited to its resonance via the injection of ultrasound waves through the investigated sample. The resonance frequencies of a cantilever in contact with a surface sample depends on the contact stiffness k* and so on the elastic properties of the sample.Attempts have been made to apply AFAM and related technique such UAFM and SNFHU for imaging the elastic properties of biological materials, however no quantitative measurements using these techniques have been reported yet. In this work we present results on the viscoelasticity of agar gel-samples as measured by AFAM. Agar gel is a good model material to test the ability of AFAM on soft mater. Further we show application examples of AFAM on biological materials (i.e. biofilms and the human periodental ligament) to investigate their viscoelastic properties.

12:10 PM
Multi-Scale Mechanisms of Osteogenesis Imperfecta Disease in Collagenous Tissues: *Markus Buehler*[1]; Alfonso Gautieri[1]; Sebastien Uzel[1]; [1]Massachusetts Institute of Technology

Osteogenesis imperfecta is a genetic disorder in collagen characterized by mechanically weakened tendon, fragile bones, skeletal deformities and in severe cases prenatal death. Here we show by a hierarchy of full atomistic and mesoscale simulation that osteogenesis imperfecta mutations severely compromise the mechanical properties of collagenous tissues at multiple scales, from single molecules to collagen fibrils. Mutations that lead to the most severe osteogenesis imperfecta phenotype correlate with the strongest effects, leading to weakened intermolecular adhesion, increased intermolecular spacing, reduced stiffness, as well as a reduced failure strength of collagen fibrils. Our findings provide insight into the microscopic mechanisms of this disease and lead to explanations of characteristic osteogenesis imperfecta tissue features such as reduced mechanical strength and lower cross-link density. The study explains how single point mutations can lead to catastrophic tissue failure at much larger length-scales, and makes a direct links between genetics, mechanical failure, and material properties.

Bulk Metallic Glasses VII: Fatigue and Corrosion

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee
Program Organizers: Peter Liaw, The University of Tennessee; Hahn Choo, The University of Tennessee; Yanfei Gao, The University of Tennessee; Gongyao Wang, University of Tennessee

Wednesday AM Room: 213
February 17, 2010 Location: Washington State Convention Center

Session Chairs: D. Gary Harlow, Lehigh University; Annett Gebert, Leibniz-Institute for Solid State and Materials Research IFW Dresden

8:30 AM Invited
A Fracture Mechanics Model of Fatigue Crack Propagation in Bulk-Metallic Glasses: Xiaoqing Jin[1]; *Leon Keer*[1]; Gongyao Wang[2]; Peter Liaw[2]; [1]Northwestern University; [2]The University of Tennessee

A three-point bending experiment was performed to investigate the fatigue behavior of Zr50Cu40Al10 bulk metallic glass (BMG). The fatigue crack growth path as well as both the fine and coarse fatigue striation spacings were measured during the testing. In amorphous alloys, since the crystal defects are absent and plastic flow is mainly confined to the shear bands, their formation could play a significant role in causing fracture. It is postulated that a fatigue crack initiates from the ruptured shear band, and advances conforming to the shear bands along the most favorable direction. A modeling analysis implementing the energy criterion of linear elastic fracture mechanics (LEFM) is developed to explore the proposed fatigue mechanism based on the shear band hypothesis. The present numerical simulation predicts good agreement with the fatigue crack characteristics observed in the experiments.

8:50 AM
Mechanisms of Fatigue Crack Growth in Zr-Based Bulk Metallic Glasses: *Jamie Kruzic*[1]; Sarah Philo[1]; Maximilien Launey[2]; [1]Oregon State University; [2]Lawrence Berkeley National Laboratory

Fatigue crack growth rates were measured for $Zr_{44}Ti_{11}Ni_{10}Cu_{10}Be_{25}$ and $Zr_{58.5}Nb_{2.8}Cu_{15.6}Ni_{12.8}Al_{10.3}$ bulk metallic glasses (BMGs). Growth rate data overlapped considerably for both. To understand the mechanisms of fatigue crack growth the former BMG was tested in different initial free volume and residual stress states, and in both an ambient air and dry nitrogen environment. Fatigue crack growth rates were relatively unaffected by the initial free volume state. This was attributed to the formation of a fatigue transformation zone of increased local free volume at the fatigue crack tip. When residual thermal tempering stresses from the initial processing were not annealed out, it was found that the fatigue threshold and fracture toughness were both increased due to residual compressive stresses at the sample surfaces suppressing crack growth. Finally, it was found that testing in a dry nitrogen environment significantly increased the fatigue threshold, suggesting a corrosion fatigue mechanism in ambient air.

9:00 AM Invited
Effect of Stress Gradient on Fatigue Strength of Zr-Based Bulk Metallic Glass: *Yoshikazu Nakai*[1]; Kohei Fujihara[1]; Naoki Sei[1]; Kunihiro Ando[1]; Bok-Key Kim[2]; [1]Kobe University; [2]Myongji College

Fatigue strength of notched specimen and smooth specimen of Zr-based bulk metallic glass were conducted under either plane-bending or axial-loading. The fatigue notch factor was almost equal to the elastic stress concentration factor either for plane-bending or for axial loading. It indicates that the effect of stress gradient around notch root is negligible, and the fatigue limit of notched specimen is determined by the stress at the notch root. On the contrary, the fatigue strength and the fatigue limit were lower for the axial-loading than the plane-bending either for notched or smooth specimen. It is considered that the fatigue strength of BMG depends on the cooling rate in the casting process of the material, which is different along the thickness direction, and the fatigue strength of plane-bending reflects the strength at the specimen surface while that of axial-loading is determined by the weakest strength in the thickness direction.

9:20 AM

Near-Threshold Fatigue Crack Growth in Metallic Glass Matrix Composites: Kombaiah Boopathy[1]; *Douglas Hofmann*[2]; William Johnson[3]; Upadrasta Ramamurty[1]; [1]Indian Institute of Science; [2]Liquidmetal Technologies; [3]California Institute of Technology

A major drawback in using bulk metallic glasses (BMGs) as structural materials is their extremely poor fatigue performance. One way to alleviate this problem is through the composite route, in which second phases are introduced into the glass to arrest crack growth. In this work, the fatigue crack growth behavior of in-situ reinforced BMGs with crystalline dendrites, which are tailored to impart significant ductility and toughness to the BMG, was investigated. Three composites, all with equal volume fraction of dendrite phases, were examined to assess the influence of chemical composition on the near threshold fatigue crack growth characteristics. Nanoindentation experiments on the constituent phases show that the amorphous matrix is much harder and stiffer as compared to the crystalline dendritic phase. The threshold stress intensity factor range for fatigue crack initiation in composites was found to be enhanced by more than 100%.

9:30 AM Invited

Fracture and Fatigue of Zr- and Ti-Based Metallic Glass In-situ Matrix Composites: *Maximilien Launey*[1]; Douglas Hofmann[2]; William Johnson[2]; Robert Ritchie[3]; [1]Lawrence Berkeley National Laboratory; [2]California Institute of Technology; [3]University of California Berkeley

The mechanical properties of bulk metallic glasses (BMGs) are often plagued by low fracture and fatigue resistance. Correspondingly, much effort in recent years has been devoted to improving their damage tolerance properties, either through compositional changes or by introducing some degree of microstructure. By matching the microstructural length scales (of a second phase) to mechanical crack-length scales, metallic glass matrix composites demonstrate strongly improved tensile ductility, fracture toughness, and fatigue resistance. These remarkable improvements are explained by the effect of the mechanically soft and ductile second phase, which acts stabilizing against shear localization and critical crack propagation; it results in extensive plastic shielding, which further stabilizes crack growth. The fracture and fatigue behavior of semi-solidly processed Zr- and Ti-based BMG matrix composites with in-situ dendritic phase was examined. Specifically resistance-curve, fatigue crack-growth, and stress-life behavior are here presented in light of the relevant toughening and fatigue mechanisms involved.

9:50 AM

Effects of Laser-Surface Modification on Bending-Fatigue Characteristics of Zr-Based Bulk Metallic Glasses: *Ritesh Sachan*[1]; G.Y. Wang[1]; P.K. Liaw[1]; Ramki Kalyanaraman[1]; [1]University of Tennessee-Knoxville

For the last two decades, bulk metallic glasses (BMGs) have received attention from material science community because of their unusual characteristics, including high tensile strengths and great elastic limits. Recently, much work has focused on studying the inherent brittleness of BMGs. Here we investigate the surface modification of Zr50Cu30Al10Ni10 metallic glass by nanosecond pulsed laser irradiation. Surface treatments were performed as a function of laser-energy density, number of pulses, and spatial uniformity of laser beam (i.e., interference irradiation). The resulting surface structure and morphology was investigated by the scanning-electron microscopy (SEM), atomic-force microscopy (AFM), and x-ray diffraction techniques. The resulting surface structure and morphology was correlated with 4-point bending experiments to measure the bending fatigue properties of bar-shaped specimens. A significant change was observed in number of cycles to failure at a constant stress range, suggesting that the surface-laser treatment could help control the fatigue behavior of BMG specimens.

10:00 AM Break

10:10 AM Invited

Statistical Aspects of Fatigue for Bulk-Metallic Glasses: *D. Gary Harlow*[1]; Gongyao Wang[2]; Peter Liaw[2]; Yoshihiko Yokoyama[3]; [1]Lehigh University; [2]University of Tennessee; [3]Tohoku University

The fatigue lives of bulk-metallic glasses (BMG) exhibit large scatter. The primary sources are from manufacturing, microstructure, environment, and loading. Because of the inherent microstructural properties of BMG, experimental testing cannot adequately identify all of the sources and magnitude of the randomness in the fatigue life. Nevertheless, the identification and significance of these variables are paramount for predicting the fatigue life. The variability associated with differences in fatigue-testing techniques, manufacturing processes, material properties, and chemical compositions are investigated. The statistical characterization of internal inhomogeneities and surface damage, each of which impact fatigue lives, is considered. Three classes of BMG, i.e., Zr, Cu, and Fe based BMG, are examined to study the statistical effect of different microstructures. Also, the statistical influence of cast processing is investigated by considering two different processes. The statistical properties are examined in the context of standard stress and fatigue-life cycles (S-N) response.

10:30 AM

Zr-Base Glass-Forming Film for Fatigue Property Improvements of 316L Stainless Steel: Jinn Chu[1]; *Cheng-min Lee*[1]; Peter Liaw[2]; [1]Nation Taiwan University of Science and Technology; [2]The University of Tennessee

Effects of 200-nm-thick glass-forming $Zr_{53}Cu_{29}Al_{12}Ni_6$ sputtered film on four-point bending fatigue properties of 316L stainless steel substrate have been investigated. The fatigue life is found to improve from $4.4x10^5$cycles of uncoated sample to $4.5x10^6$ cycles of coated sample under a stress of 750MPa. The life is further increased to $>10^7$ cycles, more than 22 times, when the film is annealed in supercooled liquid region (ΔT). The improvements in fatigue limit are 700MPa and 750MPa for as-deposited and annealed films, respectively, from 600MPa of uncoated sample. The excellent fatigue properties are attributed to the several factors, such as smooth surface, high film strength and better adhesion between film and 316L stainless steel. The sample surface becomes smooth after coated with the film, and it is further improved after annealing in ΔT. As a result, the substrate with the annealed film could have enhanced fatigue properties. Detailed results will be presented.

10:40 AM Invited

Effect of Surface Finishing and Mechanically Induced Defects on the Corrosion of Bulk Metallic Glasses: *Annett Gebert*[1]; [1]Leibniz-Institute for Solid State and Materials Research IFW Dresden

It is well established that surface reactivity and corrosion behaviour of amorphous alloys is principally determined by various material-dependent factors. it is clearly demonstrated that under real casting and rapid quenching conditions the preparation of absolutely defect-free amorphous alloys is nearly impossible. The paper reports on first systematic studies regarding the effect of different mechanically and chemically generated surface finishing states on the anodic behaviour of Zr-based bulk metallic glasses. It will be demonstrated that depending on the treatment process the active –passive behaviour can be significantly altered. Fundamental studies combining electrochemical and surface analyses with mechanical testing of selected Zr-based bulk glass-forming alloys were conducted. Those clearly revealed that the pitting initiation is dependent on the mechanically induced defect concentration. Pits are pinned to pre-formed shear bands at the sample surface. The stress field of local mechanical defects supports the corrosion process and determines the corrosion damage morphology.

11:00 AM

Fatigue Behavior of Tough Fe-Based Bulk-Metallic Glasses: *Gongyao Wang*[1]; Marios Demetriou[2]; Russell Graves[1]; Peter Liaw[1]; William Johnson[2]; [1]University of Tennessee; [2]California Institute of Technology

Amorphous steel alloys of composition Fe-(Mo,Ni,Cr)-(C,B)-P with low shear moduli exhibiting high toughness and good glass-forming ability have recently been developed. Specifically, alloy Fe70Mo5Ni5C5B2.5P12.5 forms glassy rods 4 mm in diameter, has a shear modulus of 57 GPa, and exhibits notch toughness of 50 MPa×m1/2. In this presentation, results from compression-compression fatigue experiments performed on Fe70Mo5Ni5C5B2.5P12.5 in air will be introduced. The applied stress versus cycles to failure (S-N) curve will be presented and compared to other Fe-based and Zr-based bulk-metallic glasses. Moreover, a mechanistic insight into the mechanism governing the fatigue failure in a low-shear-modulus high-toughness Fe-based bulk-metallic glasses will be proposed. The present work is supported by the National Science Foundation (NSF), the Combined Research-Curriculum Development (CRCD) Program, under EEC-9527527 and EEC-0203415, the Integrative Graduate Education and Research Training (IGERT) Program, under DGE-9987548, the International Materials Institutes (IMI) Program, under DMR-0231320.

11:10 AM Invited
Stress-Assisted Corrosion of Cu-Based Bulk Metallic Glass: Ding Li[1]; *Fuqian Yang*[1]; Peter K. Liaw[2]; [1]University of Kentucky; [2]University of Tennessee

Using microindentation, the stress-assisted-electrical corrosion of Cu-based bulk metallic glass (Cu46.25Zr45.25Al7.5Er1) was studied in a 10 wt% NaCl electrolyte. The microindentation was performed in an indentation load range of 500 mN to 4000 mN to create shear bands over the deformation zone. Electric current of various densities was passed through the indented-bulk metallic glass to evaluate the effect of shear bands on the electrical corrosion of the bulk metallic glass. Surface corrosion (the formation of pits) always initiated from the shear-banding zones, and the size of the corrosion zone grew with the corrosion time surrounding the shear-banding zones. Worm-like structures were formed, and the density of the worm-like structures increased with the current density and the corrosion time.

11:30 AM
Biocompatibility of Zr-Based Bulk Metallic Glasses: Effects of Micro-Alloying and Surface Roughness: *Lu Huang*[1]; Zheng Cao[2]; Wei He[2]; Harry Meyer[3]; Peter Liaw[2]; Elena Garlea[4]; Shujie Pang[1]; Tao Zhang[1]; [1]Beijing University of Aeronautics and Astronautics; [2]University of Tennessee, Knoxville; [3]Oak Ridge National Laboratory; [4]Y12 National Security Complex

The present work evaluated the effects of micro-alloying and surface roughness on the biocompatibility of Zr-based bulk metallic glasses (BMGs), and assessed their potential application as an implant material. Ti-6Al-4V alloy was selected as a reference material. Surface properties, including surface composition, surface roughness, and wettability were characterized for all substrates. Bone-forming mouse MC3T3-E1 pre-osteoblastic cells were used to investigate cellular behaviors, including cell attachment, proliferation, and differentiation activities on substrates with different compositions and surface roughness. Cell adhesion and proliferation behaviors were found comparable on all substrates. However, cell differentiation behaviors were found to be influenced by both composition and roughness. A higher differentiation activity was found on BMG samples than on the Ti-alloy. This study concluded that, in addition to their excellent mechanical and electrochemical properties, Zr-based BMGs exhibited a good biocompatibility which made them a competitive candidate to be used as a medical implant material.Acknowledgement: This work was supported by the International Materials Institutes (IMI) program, and the National Natural Science Foundation of China (NSFC).Research at the Oak Ridge National Laboratory SHaRE User Facility was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

11:40 AM
Compression-Compression Fatigue Behavior of Zr-Based Bulk-Metallic Glasses: *Gongyao Wang*[1]; P. Liaw[1]; Y. Yokoyama[2]; R. Graves[1]; A. Inoue[2]; [1]University of Tennessee; [2]Institute for Materials Research

Rod Zr50Cu40Al10, Zr60Cu30Al10, and Zr50Cu30Al10Ni10 (in atomic percent) bulk-metallic glasses (BMGs) were fabricated by an arc-melt tilt-casting technique. Compression-compression fatigue experiments were performed on these zirconium (Zr)-based BMGs in air. The experiments were conducted at a frequency of 10 Hz, using an electrohydraulic machine with an R ratio of 0.1, where R = |s|min./|s|max., |s|min. and |s|max. are the applied minimum and maximum absolute stresses, respectively. These samples exhibit high fatigue-endurance limits of over 1,400 MPa, based on the stress range. The results suggested that the fatigue resistance of BMGs can be improved with fabrication technique. A mechanistic understanding of the compression-compression fatigue behavior of these Zr-based BMGs is provided. The present work is supported by the National Science Foundation (NSF), the Combined Research-Curriculum Development (CRCD) Program, under EEC-9527527 and EEC-0203415, the Integrative Graduate Education and Research Training (IGERT) Program, under DGE-9987548, the International Materials Institutes (IMI) Program, under DMR-023132

11:50 AM Invited
Corrosion Behaviors of Fe41Co7Cr15Mo14C15B6Y2 Bulk Metallic Glass in Sulfuric Acid Solutions: *Jun Shen*[1]; [1]Harbin Institute of Technology

The corrosion resistance of Fe41Co7Cr15Mo14C15B6Y2 bulk metallic glass in sulfuric acid solutions was determined by electrochemical measurement. The passive film formed on the surface of the alloy after immersion in the 0.5 mol/L H2SO4 solution for a week was analyzed by X-ray photoelectron spectroscopy (XPS). Electrochemical measurements show that the corrosion resistance of the studied alloy in the 1 mol/L H2SO4 solution is superior to stainless steel (SUS 321), and almost the same as Ti6Al4V, indicating that the amorphous alloy studied exhibits excellent corrosion resistance in sulfuric acid solutions.

Cast Shop for Aluminum Production: Direct Chill and Conveyor Casting

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee, TMS: Aluminum Processing Committee
Program Organizers: John Grandfield, Grandfield Technology Pty Ltd; Pierre Le Brun, Alcan Voreppe Research Center

Wednesday AM Room: 609
February 17, 2010 Location: Washington State Convention Center

Session Chair: Gerd-Ulrich Grün, Hydro Aluminium Deutschland GmbH

8:30 AM
Microsegregation of Direct Chill Ingot of Super High Strength Aluminum Alloy Cast from Heavily Electromagnetically Stirred Melt: *Takateru Umeda*[1]; Pramote Thirathipviwat[1]; Mawin Suparadist[1]; Hiromi Nagaumi[2]; [1]Chulalongkorn University; [2]Nippon Light Metal

Low frequency electromagnetic casting (LFEC) applied to Al alloys produces intensive stirring in direct chill (DC) melt, which prevents hot cracking of high strength aluminum alloys never produced by DC. For instance, Al-10%Zn-2.7%Mg-2.3%Cu alloy, of which extruded and heat treated alloy shows 780MPa in tensile strength and 13% in elongation, is available by LFEC because of fine grain size due to heavy stirring and its grain size is small enough, such as $45*10^{-6}$ m cast into 200 mm diameter billet.Not only to control this new casting well but also to develop alloy designing properly it is necessary to understand solidification behavior microscopically. Therefore, in this report, microsegregation in accordance with solidification progress including formation of various kinds of intermetallic compounds is firstly discussed by both precise experiments and the prediction by using thermodynamic data base. Next solute redistribution is simulated considering back diffusion happened by fine grain size.

8:55 AM
Utilizing Safety Pit Coating Repair Kits to Prevent Production Stoppages: *Alex Lowery*[1]; Joe Roberts[2]; [1]Wise Chem LLC; [2]Pyrotek Inc.

Studies have proven that safety pit coatings prevent molten metal explosion from bleed-outs during direct chill casting in an aluminium mills. The safety pit coatings are applied to any substrate that can come into contact with any molten metal at the casting station. Upon repeated exposures the coating surface sacrifices itself upon contact with molten metal to prevent an explosion from occurring. Eventually the coating surface exposes the bare substrate (e.g., concrete, steel, stainless steel). Further studies have shown that a bare spot as small as 4 sq. inches (25.4 sq. cm) in the safety pit coating surface can be an ignition source for a molten metal explosion.Repair of the damaged coating surface was time consuming and commonly disrupted production. Recent introduction have safety pit coating repair kits that enable the quick repair of damaged coating surfaces have minimized and in most instances eliminated any disruption in production.

9:20 AM
Effect of Application of out-of-Phase Electromagnetic Field on Horizorntal Direct Chill Casting of 7075 Aluminum Alloy: *Qingfeng Zhu*[1]; Zhihao Zhao[1]; Xiangjie Wang[1]; Jianzhong Cui[1]; [1]Key Laboratory of Electromagnetic Processing of Materials, Ministry of Education, Northeastern University

The effect of application of the out-of-phase electromagnetic field in HDC on the process and the metallurgical quality of 7075 alloy ingots was investigated in detail. The results show that when out-of-phase electromagnetic field was applied, the effect of gravity on the HDC casting process was eliminated effectively, the temperature distribution in the pool became more uniform, the cooling difference between upper and bottom surface and depth of sump were decreased, the sump shape was changed to be more symmetric about geometrical center of the mold, the thickness of segregation layer decreased and the surface quality and the microstructures of the ingots were improved, the area of feathery grains decreased and the area of equiaxed grains increased, the equiaxed grains were refined and the floating grains eliminated so that the quality of the ingots was improved.

9:45 AM
Next Generation of Almex Direct Chill Tooling Systems: *Shaun Hamer*[1]; [1]Almex USA Inc.

Almex USA Inc. has introduced the next generation of slab and rolling ingot tooling systems for Direct Chill casting of aluminum alloys. The design is based upon the Almex philosophy of 'Safety, Simplicity and Performance". The new systems are a result of extensive thermodynamic, fluid dynamic and metallurgical modeling combined with decades of cumulative design experience and hands-on casting knowledge and understanding. The result is a tooling system with a wide operating window allowing for excellent process and alloy flexibility. Combining this tooling with Almex proprietary casting recipes and practices facilitates the end user with the capability of producing world class slab and rolling ingot with excellent metallurgical properties, high pit recovery and optimum safety for casting of alloys across the entire wrought alloy series. This paper describes the key design features of this new tooling and provides evaluation of the metallurgical and process performance of the system.

10:10 AM
Thermal Assessment of the Casting Operation at IMASA Shop: Claudio Méndez[1]; César Sánchez[1]; Gabriel Plascencia[1]; Marco Rubio[2]; *David Jaramillo*[1]; [1]CIITEC - IPN; [2]IMASA S.A. deC.V.

A thermal assessment of the semi-continuous casting facility at IMASA shop was conducted. Temperature measurements were carried out in situ as ingots of the 1XXX and 3XXX aluminum alloys series were processed. Simultaneously, the temperature in the cooling water was measured and recorded. With the data collected at the shop, a thermal balance was performed. It was found that there is a significant excess in the amount of water used for heat extraction during the solidification of the ingots. This major finding; lead to conceptualize a more efficient cooling system, since the current cooling system increase the production cost at IMASA. This new cooling system concept is under development and some first results obtained from finite element analysis are presented and discussed in this paper.

Characterization of Minerals, Metals and Materials: Characterization of PMC's, Composites, Fibers, Polymers, and Organics

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division, TMS Structural Materials Division, TMS/ASM: Composite Materials Committee, TMS: Materials Characterization Committee
Program Organizers: Ann Hagni, Geoscience Consultant; Sergio Monteiro, State University of the Northern Rio de Janeiro - UENF; Jiann-Yang Hwang, Michigan Technological University

Wednesday AM | Room: 307
February 17, 2010 | Location: Washington State Convention Center

Session Chairs: Mingdong Cai, Exova; Jeong Guk Kim, Korea Railroad Research Institute

8:30 AM
Weibull Analysis of Tensile Tested Piassava Fibers with Different Diameters: Denise Cristina Nascimento[1]; Ludy Motta[1]; *Sergio Monteiro*[1]; [1]State University of the Northern Rio de Janeiro - UENF

Technical and economical advantages in addition to environmental considerations are promoting the substitution of natural fiber for the glass fiber in polymer matrix composites. However, by contrast to the glass fiber uniformity, natural fibers are heterogeneous in their dimensions, especially the cross section measured by the equivalent diameter. It has been found that this variability in diameter can be correlated to different levels of mechanical resistance. In this work, a statistical analysis of tensile strength of piassava fibers using the Weibull methodology was performed. An attempt to correlate the fiber strength, obtained in tensile tests, with the diameter, precisely measured by means of a profile projector, was carried out. The results revealed an inverse dependence between the piassava fiber diameter and corresponding tensile strength. Fracture tip observation by SEM suggested possible mechanisms that could justify this inverse correlation.

8:50 AM
Thermal Analysis of Curaua Fiber Reinforced Polyester Matrix Composites: Ailton Ferreira[1]; Ruben Jesus Rodriguez[1]; Felipe Lopes[1]; *Sergio Monteiro*[1]; [1]State University of the Northern Rio de Janeiro - UENF

Natural fiber reinforced polymer composites are gaining attention as an environmentally correct solution to replace glass fiber composites. Among the drawbacks associated with the application of natural fibers, especially those lignocellulosic obtained from plants, the low thermal resistance is a limitation for composites subjected to temperatures above 100oC. The hydrophilic nature of the lignocellulosic fiber causes water evolution at this temperature level, which may introduce pores and flaws in the polymeric matrix of the composites. The objective of the present work was to conduct a thermal gravimetric analysis (TGA) on polymer composites with different amounts of curaua, a strong lignocellulosic fiber. Both TGA and DTA curves were analyzed to determine the effect of the curaua fiber on the thermal resistance of the composites. It was found that not only higher weight loss but also displacement of DTA peaks towards higher temperatures were associated with the curaua fibers in the composites.

9:10 AM
Thermographic Characterization of Damage Evolution in Polymer Matrix Composites: *Jeongguk Kim*[1]; Sung Cheol Yoon[1]; Jung-Seok Kim[1]; Hyuk-Jin Yoon[1]; Sung-Tae Kwon[1]; [1]Korea Railroad Research Institute

The tensile failure behavior of glass fiber reinforced epoxy polymer matrix composites (PMCs) was characterized using infrared camera. In order to monitor tensile damage evolution of PMC sample, a high-speed infrared camera was used to measure surface temperature changes during tensile testing. Through the thermographic image analysis, crack initiation and propagation were qualitatively monitored. Moreover, the thermographic images provided the information on fracture mode and mechanisms in PMC sample. After tensile testing, the microstructural characterization using SEM was performed on tensile fractured specimens. The SEM characterization results were comparable with in-situ monitored IR camera analysis results. In this investigation, an IR camera and SEM characterization method were used to facilitate a better understanding of damage evolution and failure mode of PMC materials during tensile testing.

9:30 AM
Characterization of the Flexural Properties of Polyester Matrix Composites Reinforced with Continuous Jute Fibers: *Sergio Monteiro*[1]; Leandro Marques[1]; Kestur Satyanarayana[2]; [1]State University of the Northern Rio de Janeiro - UENF; [2]Federal University of Parana (UFPR)

Engineering applications of natural fibers, especially those obtained from cellulose-containing plants is nowadays considered an environmentally correct alternative to substitute non-recyclable energy-intensive, abrasive and toxic synthetic fibers like the common glass fiber. Composites reinforced with lignocellulosic fibers such as coir, hemp and jute are already on the market. These composites are normally processed for short-cut fibers that do not present the highest mechanical strength as compared to continuous fibers of the same kind. The objective of this work was to study the mechanical behavior, by means of flexural tests, of polyester matrix composites reinforced with continuous jute fibers. Bend tests were conducted in standard specimens with up to 40% of jute. Fracture analysis by SEM displayed the rupture mechanisms. The results showed an improvement in some flexural properties with incorporation of jute fiber. However, a low fiber/matrix interfacial stress was responsible for limitation in the values attained by some properties.

9:50 AM
Charpy Toughness Behavior of Continuous Sisal Fiber Reinforced Polyester Matrix Composites: Wellington Inácio[1]; Felipe Lopes[1]; *Sergio Monteiro*[1]; [1]State University of the Northern Rio de Janeiro - UENF

Natural fibers obtained from plants are increasingly being applied as polymer composite reinforcement for interior automobile parts such as covers and panels. These parts should be impact resistant and absorb the energy without splitting in sharp pieces during a crash event. Sisal is a strong natural fiber that has not yet been considered for such composites. Therefore, this work investigates the toughness behavior of polyester matrix composites reinforced with up to 40% in volume of long, continuous and aligned sisal fibers by means of Charpy impact tests. It was found that the addition of sisal fibers results in a marked increase in the absorbed impact energy of the composites. Macroscopic observation of the post-impact specimens and SEM fracture analysis showed that longitudinal rupture through the sisal fiber interface with the polyester matrix is the main mechanism for the remarkable toughness of these composites.

10:10 AM
Evaluation of the Interfacial Strength of Ramie Fibers in Polyester Matrix Composites: Frederico Margem[1]; Felipe Lopes[1]; *Sergio Monteiro*[1]; [1]State University of the Northern Rio de Janeiro - UENF

The efficiency by which an applied load is transmitted through the composite structure depends on the strength of the interface between the matrix and the second phase. In fiber reinforced composites, the interfacial shear stress plays a major role in the composite capacity to support the applied load. This interfacial stress can be obtained by means of pullout tests using the fiber embedded to a certain length in a socket of the matrix material. In the present work, pullout tests were performed to evaluate the interfacial stress of ramie, a relatively strong natural fiber, reinforcing polyester matrix composites. The general result permitted to calculate a critical length for the ramie fiber embedded in polyester resin. From this critical length, the value of the interfacial stress was calculated. An interpretation of this result together with SEM observation displayed a relatively weak bond between the ramie fiber and the polyester matrix.

10:30 AM
Patterning Atop Shape Memory Polymers and Their Characterization: Y. Zhao[1]; *Mingdong Cai*[2]; Weimin Huang[1]; T. H. Tong[3]; [1]Nanyang Technological University; [2]Exova Group Ltd and Southeast University; [3]Cornerstone Research Group Inc.

The surface morphology of materials is of fundamental importance to many applications (e.g., surface wetting, friction, surface roughness, reflection, drag, adhesion, etc). Various approaches for micro/nano patterning atop polymer surfaces have been proposed in recent years. However, a cost effective technique is still highly in demand. In this paper, we demonstrate a few novel but rather simple and generic approaches for surface micro/nano patterning using shape memory polymers (SMPs). Reversible micro vertical chains, crown shaped protrusion arrays and strip/labyrinth wrinkles atop SMPs are presented. Those novel 3-D surface structures are quantitatively analyzed by scanning electron microscopy and atomic force microscopy.

10:50 AM
Characterization of a Natural Biofoam from the Buriti Palm Tree: Lucas Costa[1]; *Sergio Monteiro*[1]; Tammy Portela[1]; Nubia Santos[2]; Cecília Zavaglia[2]; [1]State University of the Northern Rio de Janeiro - UENF; [2]State University of Campinas - UNICAMP

Solid foams are non-fluid porous materials with a large capacity to retain air, which makes them lighter than the water with densities below 0.5 g/cm3. These foams are nowadays extensively used in engineering applications such as thermal insulation, packing, lifebuoy, automobile cushion, furniture and many others. Most foam materials are produced by bubbling air through a polymer while in a low viscosity state. The negative side of these synthetic foams is the CO2 contribution too global warming by means of the energy required for the foaming process. Moreover, as a non-degradable polymer, discarded synthetic foams also contribute to long term water and ground pollution. In this work, a natural foam extracted from the Amazon buriti palm tree is investigated as possible substitute for synthetic foams. The basic physical and mechanical properties of this biofilm were evaluated. Its spongelike structure was characterized by the amount of pores and morphological aspects.

11:10 AM
Characterization of Fibers from Different Parts of the Buriti Palm Tree: Tammy Portela[1]; Lucas Costa[1]; Felipe Lopes[1]; *Sergio Monteiro*[1]; [1]State University of the Northern Rio de Janeiro - UENF

Well known lignocellulosic fibers extracted from cultivated plants such as cotton, sisal, jute, coir, hemp, flax and many others have been traditionally used in simple products. These fibers are nowadays, also reinforcing composites for more technological-intensive uses as automobile interior components and civil construction panels. Less known plats like the buriti palm tree can also provide lignocellulosic fibers for composite reinforcement. However, its most commonly used fiber obtained from the leaves was recently found to have low mechanical strength. By contrast, the fibers extracted from the petiole have primarily shown a higher strength. Therefore, the objective of this work was to make a comparative characterization of the structural aspects as well as technical and mechanical properties of these two different buriti fibers. The structural aspects, both for integer and tensile-ruptured fibers were characterized by SEM. The results revealed significant differences in the microstructure and properties of the investigated fibers.

11:30 AM
Tensile Properties of Epoxy Composites Reinforced with Continuous Curaua Fibers: Felipe Lopes[1]; Ailton Ferreira[1]; *Sergio Monteiro*[1]; [1]State University of the Northern Rio de Janeiro - UENF

The curaua is a bush-like plant, similar to the pineapple, native of the Amazon region. Fibers extracted from the curaua leaves are among the strongest lignocellulosic and have been used as composite reinforcement. Characterization of these composites is being carried out for different polymer matrices and mechanical tests. The objective of the present work is to evaluate the tensile properties of composites with a specific epoxy matrix reinforced with different amounts of curaua fibers. Tensile specimens with up to 40% in volume of long, continuous and aligned curaua fibers were room temperature tested in an Instron machine. The fracture was analyzed by SEM. The results showed significant changes in the mechanical properties with the amount of curaua fibers. This was compared to other bend-tested composites with distinct matrices. The fracture analysis revealed a weak fiber/matrix interface, which could be responsible for the comparatively low performance of some properties.

11:50 AM
Characterizing the Mechanical Properties of Wax-Coated Granular Composites: *John Bridge*[1]; Michael Peterson[2]; Ryan Beaumont[3]; [1]Maine Maritime Academy; [2]University of Maine; [3]R.M. Beaumont Corporation

Triaxial compression tests at various confining pressures and temperatures, as well as tangent modulus tests using ultrasonic waves, were conducted for wax-coated granular composite materials. This material is used as a surface for Thoroughbred horse racing. The purpose of these tests is to examine how track shear strength and tangent modulus at a range of loads respond to changing temperatures. Previous work has shown that a wide range of operational temperatures are experienced which have been reproduced in the lab. Using differential scanning calorimetry, it is confirmed that these operational temperatures correspond to distinct thermal transition regions for the wax that is used to coat the sand in these surfaces. Preliminary results show that both shear strength and tangent modulus are sensitive to temperature changes with maximum strengths correlating with major DSC wax transition regions.

12:10 PM
Mechanical Behavior of Polyester Matrix Composites Reinforced with Continuous Bamboo Fibers: Lucas Costa[1]; *Sergio Monteiro*[1]; Rômulo Loiola[1]; [1]State University of the Northern Rio de Janeiro - UENF

The stem of the bamboo has been traditionally used in simple structural parts such as scaffoldings and huts. In spite of the relatively high stiffness the bamboo is limited in terms of engineering application, due to its cylindrical shape. Moreover, as any lignocellulosic material, the direct exposure of the bamboo may cause deterioration. A possible solution for both, the dimensional limitation and weather deterioration is to separate the bamboo fibers from the stem to be applied as polymer composite reinforcement. The objective of this work was to characterize individual bamboo fibers and investigate the flexural mechanical properties of polyester composites reinforced with these fibers. Specimens with up to 30% of continuous and aligned bamboo fibers added to polyester composites were bend-tested until fracture. The results showed improvement in the composite strength with a decreasing tendency for higher amounts of fibers, due to the weak interface developed with the polyester matrix.

Computational Thermodynamics and Kinetics: Phase Field, CALPHAD and Other Modeling Techniques

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Chemistry and Physics of Materials Committee, TMS/ASM: Computational Materials Science and Engineering Committee
Program Organizers: Jeffrey Hoyt, McMaster University; Dallas Trinkle, Univeristy of Illinois at Urbana-Champaign

Wednesday AM Room: 308
February 17, 2010 Location: Washington State Convention Center

Session Chair: To Be Announced

8:30 AM
A Phase Field Study on the Growth and the Interaction of Ni_4Ti_3 Precipitates in Niti Shape Memory Alloy: *Wei Guo*[1]; Ingo Steinbach[1]; Christoph Somsen[2]; Gunther Eggeler[2]; [1]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum; [2]Institut für Werkstoffe, Ruhr-University Bochum

Growth and interaction among Ni_4Ti_3 particles is studied using the multi-phase field method. A special pattern of two precipitates due to the elastic interaction among them is observed. This means that precipitates have strong elastic interaction among each other. It is also found that applied stress has a strong effect on the Ni_4Ti_3 shape. Under a compressive stress along the axis of the disc-shape precipitate, the aspect ratio increases with the applied stress up to around 1. This phenomenon agrees qualitatively with the experimental observation while the sensitivity of the shape on the external stress is largely underestimated in the simulation. The growth kinetics of the precipitate can also be influenced significantly by the applied stress. With the increase of the compressive stress along the axis of precipitate its growth velocity increases notably. All simulation results are compared with experimental observations.

8:50 AM
A Mixed-Mode Model for Precipitation in Al-Mg-Si Alloys: *Abbas Bahrami*[1]; Alexis Miroux[2]; Jilt Sietsma[1]; Leo Kestens[1]; [1]Materials Science and Engineering Department, Technical University of Delft (TuDelft); [2]Materials to Innovation Institute (M2i)

A modified Kampmann-Wagner numerical (KWN) precipitation model has been developed considering the mixed-mode character of precipitate growth. The η-parameter, which is proportional to the diffusivity of the diffusing alloying element and inversely proportional to the mobility of interface and to the radius of precipitates, is used to implement the character of precipitate growth into the kinetic model. The effects of interfacial energy, diffusivity, and interface mobility on the character and kinetics of precipitation in Al-Mg-Si system have been systematically studied. The results show that the interfacial energy has almost no effect on the precipitation character. However, diffusivity and interface mobility have significant influences on the character of precipitation. The results also show that when the alloying element is interstitial, the alloy is heavily-deformed before ageing, or precipitates are very small with coherent interface, the assumption of mixed-mode growth is more accurate than the assumption of diffusion-controlled growth.

9:10 AM
Thermodynamics, Structural Properties and Transformation Behavior of CoNiGa Alloys from First Principles: *Raymundo Arroyave*[1]; Anchalee Junkaew[1]; Andres Garay[1]; Arpita Chari[1]; Chun-Wei Yao[1]; [1]Texas A&M University

CoNiGa alloys have been receiving considerable interest due to their high temperature shape memory properties. While there have been many investigations on the mechanical and magnetic behavior of these materials, very little is known about the fundamental microscopic basis for the observed macroscopic behavior. In this work, we discuss the stability of CoNiGa-based structures as a function of composition. Thermodynamic properties of these phases including vibrational, configurational, electronic and magnetic degrees of freedom are taken into account. In addition, we investigate the nature of the martensitic transformation responsible for the observed shape memory behavior. Elastic properties as well as the behavior of phonon modes allows to elucidate the specific causes for the observed instability of the austenite phase. Linking to CALPHAD methods is done in order to predict the full ternary Co-Ni-Ga phase diagram at arbitrary composition/temperature conditions.

9:30 AM
Pressure-Induced Invar Behavior in Pd3Fe: *Michael Winterrose*[1]; Matt Lucas[1]; Alan Yue[1]; Itzhak Halevy[1]; Lisa Mauger[1]; Jorge Munoz[1]; Jingzhu Hu[2]; Michael Lerche[3]; Brent Fultz[1]; [1]Caltech; [2]NSLS; [3]HPSynC

Synchrotron x-ray diffraction (XRD) measurements, nuclear forward scattering (NFS) measurements, and density functional theory (DFT) calculations were performed on L12-ordered Pd3Fe. Measurements were performed at 300 K at pressures up to 33 GPa, and at 7 GPa at temperatures up to 650 K. The NFS revealed a collapse of the 57Fe magnetic moment between 8.9 and 12.3 GPa at 300 K, coinciding with a transition in bulk modulus found by XRD. Heating the sample under a pressure of 7 GPa showed negligible thermal expansion from 300 to 523 K, demonstrating Invar behavior. Zero-temperature DFT calculations showed a ferromagnetic ground state and several antiferromagnetic states of comparable energy at pressures above 20 GPa.

9:50 AM
Explaining the Change in Diffusion Mechanism in the Series of $L1_2$ Phases In_3R (R= Rare-Earth): *John Bevington*[1]; Matthew Zacate[2]; Gary Collins[1]; [1]Washington State University; [2]Northern Kentucky University

Recent experiments revealed a remarkable change in the mechanism of diffusion for atoms on the In-sublattice along a series of In_3R line compounds having $L1_2$ structure [Phys. Rev. Lett. 102, 155901 (2009)]. Experiments were carried out on pairs of samples with opposing boundary compositions (slightly In-rich and In-poor). Whereas light lanthanide indides (R= La, Ce, Pr, Nd) exhibited higher jump frequencies for In-rich samples, heavy lanthanide indides had higher jump frequencies for In-poor samples. Since, at given temperature, R-vacancy (In-vacancy) concentrations can only increase (decrease) monotonically with increasing In composition, it was concluded that the dominant diffusion mechanisms involve R-vacancies (In-vacancies) in the light (heavy) lanthanide indides. To explain this remarkable change in behavior, calculations of point defect energies along the entire lanthanide tri-indide series are being carried out using the full-potential, all-electron program WIEN2k, with results to be reported at the meeting.

10:10 AM
Diffusion of Interstitial and Substitutional Elements in γ/γ' Interface in Ni-Al Superalloys: A First Principles Study: *Priya Gopal*[1]; Peter Wagner[2]; Srinivasan Srivilliputhur[1]; Gregor Mori[2]; [1]University of North Texas, Denton; [2]University of Leoben

Ni-based superalloys possess desirable high-temperature properties including strength, ductility, fracture toughness as well as resistance to creep and oxidation. An important factor for strengthening mechanism is the microstructure of the alloy which consists of ordered γ'- Ni3Al precipitates within a γ (Ni-Al) matrix. In addition, a variety of substitutional and interstitial elements like Cr, Ta, Re, Ru, Ti, W, Mo, C, S etc. play a crucial role in strengthening of these alloys. It is thus important to understand the electronic structure and diffusion of these elements. Using density functional theory methods with plane-wave basis sets we determine the partitioning behavior of alloying elements in the interface. We also systematically explore the energetics and kinetics of diffusion of Cr, Mo, C, and O in the bulk and across the γ/γ'' interface. We use transition state theory combined with nudged elastic band method to determine the transition paths and diffusion activation barriers.

10:30 AM Break

10:40 AM
Modelling Ordering Phenomena in Condensed Phases: *Bo Sundman*[1]; Mauro Palumbo[2]; Suzana Fries[2]; [1]CEA; [2]Ruhr University Bochum

Ordering phenomena are a fascinating theoretical, experimental and applied scientific topic since more than one century. For simple binary system detailed models can be made but for multicomponent system Computational Thermodynamics (CT) is the only methodolgy that can be applied to combine the adquired knowledge for relevant applications. Guided by theoretical approaches and based on experimental evidence, CT uses simple models which are very powerful in simulations for materials development, in particular the recent sucessful use of DFT results in the calculation of TCP solution phases. There are no simliar theoretical methods to deal with ordering in liquid phases but models for ordering in liquids are very important This paper reviews the present models, points out the need of improvements and how they can to be used in the recently lauchedSAPIENS project for a sustaintaible thermodynamic database.

11:00 AM
Modeling of Phase Separation in Uranium-Zirconium Alloys via Monte Carlo Methods: *Benjamin Beeler*[1]; Benjamin Good[1]; Chaitanya Deo[1]; Sergey Rashkeev[2]; Maria Okuniewski[2]; Mike Baskes[3]; [1]Georgia Institute of Technology; [2]Idaho National Laboratory; [3]Los Alamos National Laboratory

U-Zr alloys are used as the fuel matrix in sodium cooled fast nuclear reactors. They have a body centered cubic structure (γ phase) that exhibits a miscibility gap at the temperature of operation. The alloy exhibits a variation in composition under operation with zirconium atoms migrating up the temperature gradient in the high temperature γ phase. We study the two phase evolution of U-Zr using a kinetic Monte Carlo (kMC) simulation which is well suited for studying diffusion-based phase transformations. We utilize an extension of the Ising model that accounts for atom transport through vacancy migration and allows a physically meaningful definition of time. The kMC simulation is linked to first-principles calculations via the implementation of local, composition-dependant values of the migration barrier energy. The short-range order, vacancy diffusion coefficient, and self-diffusion coefficients of uranium and zirconium are determined. The variance of these parameters with temperature and composition is analyzed.

11:20 AM
Thermodynamics Calculation and Phase-Field Simulation of Morphotropic Phase Boundary in (001) Bifeo$_3$ Thin Films: *Guang Sheng*[1]; Jingxian Zhang[1]; Robert Zeches[2]; Jinxing Zhang[2]; Alexander Melville[3]; Jon Ihlefeld[3]; Venkatraman Gopalan[1]; Darrel Schlom[3]; Lane.W Martin[4]; Ramamoorthy Ramesh[2]; Zi-Kui Liu[1]; Long-Qing Chen[1]; [1]The Pennsylvania State University; [2]University of California, Berkeley; [3]Cornell University; [4]Lawrence Berkeley National Laboratory

A strain-driven morphotropic phase boundary was recently observed in (001) $BiFeO_3$ thin film deposited on YAO and LAO substrates. In this study, we constructed the strain-temperature phase stability diagram for (001) $BiFeO_3$ thin film using both thermodynamic calculation and phase-field simulations. The tetragonal to distorted rhombohedral phase boundary predicted from thermodynamic analysis is consistent with the density function calculations. The predicted strain diagram and experimental observations are in very good agreement with $BiFeO_3$ films grown on LAO and YAO with -4.29% and -6.8% strains respectively. The volume fraction changes of different phases as a function of strain from phase-fieldsimulation across the morphotropic phase boundary will be also presented.

11:40 AM
CALPHAD Modeling of the Al-Cr-Ni System Supported by First Principles Calculations: *Wren Chan*[1]; Michael Gao[2]; [1]Carnegie Mellon University; [2]National Energy Technology Laboratory

Al, Cr and Ni are among the most important alloying elements in many commercial structural alloys including Ni-based superalloys and steels. However, even today there still lacks thermodynamic description of the complete Al-Cr-Ni ternary system. In this work, this ternary is thermodynamically assessed using the CALPHAD method. Two ternary compounds are reported: hexagonal and high-temperature orthorhombic [J. Alloys Compd. 460 (2008) 299]. Their energies are studied using first principles density functional theory calculations, and are integrated into CALPHAD optimization. The ternary isotherms and liquidus data are taken from the literature. The thermodynamic descriptions of all edge binaries are taken from previous reports. The calculated ternary phase diagram will be compared with available experimental data, and the impact of this work on Ni-based superalloy will be addressed.

12:00 PM
Occupancy Probability of a Sublattice of $D0_{22}$-Ni_3V in Ni-Al-V System: Determined by Microscopic Phase Field: *Jing Zhang*[1]; Houchuang Zhuang[1]; Zheng Chen[1]; [1]Northwestern Polytechnical University

In this paper, a sublattice of $D0_{22}$-Ni_3V is subdivided into a1 and a2 according to the location they reside. We use an atomic-scale microscopic phase field to study the occupancy probabilities (OP) of a1 and a2, including antisite defect, substitutional defect and phase transition. The results are as follows: Antisite defect (V_{a1}, V_{a2}) and substitutional defect (Al_{a1}, Al_{a2}) coexist in both a1 and a2, and the sequence of OP ranked in magnitude is Ni_{a1}, Ni_{a2}, V_{a2}, Al_{a2}, V_{a1}, and Al_{a1}. The inherent atom (Ni_{a1}, Ni_{a2}) decline but defects rise with the elevated temperature. At temperature lower than 1150K, part of the being substituted Ni exchanges V on ß sublattice and the other dissolves into matrix or enters L12 structure, while at temperature higher than 1150K the being substituted Ni together with Ni from matrix enters ß sublattice, which accounts for the complicated phase transition from $D0_{22}$ to $L1_2$.

12:20 PM
Kinetic Monte Carlo Study of Sputter-Induced Morphological Patterns in Alloy Surfaces: *Bharathi Srinivasan*[1]; Ramanarayan Hariharaputran[1]; [1]Institute of High Performance Computing

Ion beam sputtering of surfaces gives rise to interesting nanopatterns. In single phase systems, these patterns form as a result of the competition between erosion by ion bombardment and surface diffusion. In the case of alloys, interesting patterns characterized by variation in both surface height and composition are formed because of the composition-dependence of surface diffusion and sputter yield.To study these rich patterns formed on alloy surfaces we have used Kinetic Monte Carlo method. In our study we find that for binary alloys the morphological patterns are accompanied by compostional segregation. We have characterized these patterns as a function of parameters such as flux of the ion beam, temperature, sputter yields and diffusivities of the two species and we present these results in this talk.

Cost-Affordable Titanium III: Creative Processing and Property Enhancement I

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS: Titanium Committee
Program Organizers: M. Ashraf Imam, Naval Research Lab; F. H. (Sam) Froes, University of Idaho; Kevin Dring, Norsk Titanium

Wednesday AM — Room: 618
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Curt Lavender, Pacific Northwest National Laboratory; Vasisht Venkatesh, TIMET Inc

8:30 AM
Development Pathways to Low-Cost Engineering Beta Gamma TiAl Alloys: *Young-Won Kim*[1]; [1]Development Pathways to Low-Cost Engineering Beta Gamma TiAl Alloys

Gamma (titanium aluminide) alloys possess an attractive combination of low density and high temperature (over 800°C) capability, ideal for hot structures and turbine engine components. Yet, the alloys have not been inserted into aerospace service due to their material and manufacturing limitations, which include processing difficulties requiring costly multi-step forming process and large lamellar grains lowering damage tolerance. To remove or reduce such barriers, we have explored a new class of TiAl-based alloys, called beta gamma, utilizing the beneficial effects of beta solidification on grain refinement and beta phase distribution on processibility. Tests indicate that remarkably improved processibility and machinability, along with required attributes, could be achieved on the composition that would yield a desired phase distribution as a function of temperature. This presentation discusses our ongoing effort in optimizing the beta gamma alloy composition and processing, which will be led to a low-cost viable structural materials technology.

8:55 AM
Microstructure and Mechanical Properties of A' Martensite Type Ti-V-Al Alloy after Cold- or Hot Working Process: *Hiroaki Matsumoto*[1]; Hiroshi Yoneda[1]; Kazuhisa Sato[1]; Toyohiko Konno[1]; Akihiko Chiba[1]; [1]Institute for Materials Research, Tohoku University

Ti alloys are widely used for industrial applications due to their excellent mechanical properties combined with low density. In general, Ti alloys are classified as a, a+ß and ß alloys. Quite recently, we have presented new type structural a' martensite Ti alloys with low Young's modulus, high strength and excellent ductility at room temperature. Microstructural control technique utilizing a' martensite is not so common in industrial production of Ti alloys. Therefore, there have been few reports concerning the systematic characteristic with martensite (a' or a") structure. In this work, we examined the microstructure and mechanical properties of a' martensite type Ti-V-Al alloy after cold- or hot working process. Then, we found that refined equaxed (a+ß) microstructure with grain size less than 1 µm was obtained by hot working with starting structure of a' martensite. This result suggests the new type deformation processing utilizing a' martensite in industrial Ti alloys.

9:20 AM
Effect of Oxygen on Phase Precipitation and Mechanical Functionality in Ti-29Nb-13Ta-4.6Zr: *Mitsuo Niinomi*[1]; Masaaki Nakai[1]; Toshikazu Akahori[1]; Harumi Tsutsumi[1]; [1]Tohoku University

From the viewpoint of saving resources of rare metals, proper using common metals such as Fe, Si, Cu and Sn or interstitial elements such as O, N, C and H, which have been regarded as impurities in titanium and its alloys, as alloying elements to improve the mechanical functionalities of titanium alloys is becoming more important. Among those elements, oxygen plays very important roles in titanium and its alloys. Solute oxygen in titanium alloys leads to solid solution strengthening, suppressing the precipitation of the athermal omega or orthorhombic martensite phase, enhancing the formation of the alpha-case, etc. The proper using oxygen is effective to improve the mechanical functionalities of titanium alloys. However, the role of oxygen in titanium alloys is still not well understood. Therefore, the effect of oxygen on the mechanical functionalities such as strength-ductility balance, Young's modulus and super elastic behavior in Ti-29Nb-13Ta-4.6Zr was investigated.

9:45 AM
Local Heat Treatment of Titanium Alloys: Microstructure and Mechanical Properties: *Pavlo Markovsky*[1]; [1]G.V. Kurdyumov Institute for Metal Physics, NAS of Ukraine

Local Rapid Heat Treatment (LRHT) based on induction-heating methods can be used to form unique location-specific microstructures and properties in commercial titanium alloys while maintaining the bulk of the material in an initial, non-heat-treated condition. The present work focused on commercial-purity titanium (CP-Ti), Ti-6Al-4V, and TIMETAL-LCB. For each alloy, LRHT was performed using cylindrical specimens of 8 mm diameter that were surface heated to temperatures up to 1000oC at a rate of approximately 400oC/s followed by water quenching. By and large, the treatments produced a significant improvement in tensile and fatigue strength and a decrease in ductility. The source of these changes in properties will be discussed in terms of the evolution of microstructure and phase composition as well as residual stresses formed in surface layers, each of which depended on the specific alloy.

10:10 AM Break

10:25 AM
The Relative Contribution of Factors Influencing the Flow and Thermal Fields in Electron Beam Casting of Ti-6Al-4V: Tao Meng[1]; *Daan Maijer*[1]; Steven Cockcroft[1]; Riley Shuster[1]; Denis Favez[1]; David Tripp[2]; Stephen Fox[3]; [1]The University of British Columbia; [2]TIMET Morgantown; [3]TIMET Henderson

Electron Beam Cold Hearth Remelting/Melting is a relatively new and cost-effective consolidation technique for titanium alloys. The flow field that develops within the ingot liquid pool in the associated casting process is influenced by several factors including buoyancy, surface tension (Marangoni) phenomena and the decreasing permeability within the mushy zone; the former two tending to drive flow whereas the latter tends to attenuate the flow. In this study, a coupled thermal-fluid flow model of a Ti-6Al-4V electron beam button melting process has been developed to examine the relative contribution of these factors on the temperature distribution, flow field, and pool profile. Additionally, an approximation of the time-dependent electron beam pattern by a time-averaged heat source has been evaluated. It is shown that above a critical pattern repetition frequency, the surface temperature field can be correctly calculated with this time-averaged approximation, thus reducing drastically computation time.

10:50 AM
The Influence of Surface Treatments and Subsequent Annealing on the Fatigue Performance of Ti-6Al-4V for Biomedical Applications: Milos Janecek[1]; Jaroslav Fencl[2]; Lothar Wagner[3]; Robert Kral[1]; *Josef Strasky*[1]; [1]Charles University; [2]Beznoska, Ltd.; [3]Clausthal University of Technology

Alpha-beta titanium alloys, in particular Ti-6Al-4V, are widely used as surgical implant materials for large-sized joint replacements such as artificial knee, hip and shoulder. Electro-erosion was performed to prepare the surface of the alloy for optimum bone cell growth. However, tensile properties and in particular fatigue performance were found to markedly suffer from this treatment. For example, yield stress, ultimate tensile strength, tensile ductility and fatigue strength were decreased to values unacceptable for biomedical applications. In order to improve these properties, various further treatments including annealing after electro-erosion were conducted. Changes in properties will be correlated with modifications in microstructure as observed by optical microscopy and SEM.

11:15 AM
Microstructure-Properties of Cast Ti-5Al-5Mo-5V-3Cr with Elevated Oxygen Levels: *Edward Chen*[1]; D. R. Bice[1]; J. A. Hall[2]; [1]Transition45 Technologies, Inc.; [2]Wah Chang

Alloy Ti-5Al-5Mo-5V-3Cr-0.5Fe (Ti-5553) is an emerging high strength titanium alloy with improved mechanical properties compared with the industry workhorse Ti-6Al-4V. It is primarily targeted for aerospace applications including as airframe structures. All works to date on Ti-5553 have focused on more costly aerospace grades that may not be suitable for non-aerospace applications. For cost sensitive systems such as combat vehicles and armaments, a lower cost Ti-5553 with higher oxygen levels may be preferable. This work evaluates the microstructure-properties of cast Ti-5553 with oxygen levels above the maximum specified in aerospace standards. Casting is chosen here since the ability to produce complex shapes near-net offers additional cost and weight savings over traditionally machined wrought components. Mechanical properties of the "non-aerospace" Ti-5553 castings are discussed in relation to their aerospace grade counterparts, and show outstanding strength and ductility even at elevated oxygen levels. This work was supported by the U.S. Army-ARDEC.

11:40 AM
Elevated-Temperature Fatigue Behavior of Boron-Modified Ti-6Al-4V: *Wei Chen*[1]; Carl Boehlert[1]; Jane Howe[2]; Seshacharyulu Tamirisakandala[3]; Daniel Miracle[4]; [1]Michigan State University; [2]Oak Ridge National Lab; [3]FMW Composite Systems Inc.; [4]US Air Force

This work investigated the elevated-temperature fatigue behavior of Ti-6Al-4V(wt.%) modified with 1B. The fatigue response of alloys in four different product forms, namely, ingot casting (IC), IC plus extrusion, powder metallurgy (PM) rolled plate, and PM extrusion, at 455°C and a maximum applied stress range of 250-700 MPa (R=0.1, 5Hz) was compared. The PM alloys exhibited microstructures containing equiaxed grains while the IC alloys contained α+β lath microstructures, which enabled the PM alloys to achieve greater fatigue lives than the IC processed alloys. In both the PM extruded and IC extruded alloys, the TiB whiskers were aligned in the extrusion direction and the α-phase was strongly textured with the basal plane predominately oriented perpendicular to the extrusion axis. The equiaxed α+β microstructure and the α- and TiB-phase textures were identified to be responsible for the significantly higher fatigue strength exhibited by the PM extruded alloy compared to the other conditions.

Electrode Technology for Aluminum Production: Anode Green Mill

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee
Program Organizers: Ketil Rye, Alcoa Mosjøen; Morten Sorlie, Alcoa Norway; Barry Sadler, Net Carbon Consulting Pty Ltd

Wednesday AM   Room: 616
February 17, 2010   Location: Washington State Convention Center

Session Chair: Lorentz Lossius, Hydro Aluminium AS

8:30 AM Introductory Comments

8:35 AM
Use of Eddy Current Separator in Butts Processing: *Juraj Chmelar*[1]; Hogne Linga[1]; [1]Hydro

Installation of Eddy Current Separator in a butts separation line has so far showed very promising potentials in an application in this field of industry. This equipment is able to separate aluminium and iron particles from the crushed butts. The separator has low maintenance cost and with its simple construction and small dimensions it can easily be installed in a production line. Butts can contain iron (about 0.01 wt%) and aluminium (about 0.003 wt%) particles. The total amounts are not significant, but significant enough for equipment to be damaged, with consequent loss of production, higher maintenance cost and also contamination of produced anodes. The separated aluminium showed above 95 wt% content aluminium and 3.2 wt% iron.The separator treats the +20 mm fraction. Without separation metal pieces will tend to cycle between the cone crusher and the screen until they are worn down to a size passing the upper screen.

9:00 AM

From Technology Development to Successful Start-Up and Operations of Sohar: The Potential of the Bi-Eirich Mixing Line: François Morales[1]; Magali Gendre[1]; *Nigel Backhouse*[1]; Berthold Hohl[2]; David Stephenson[3]; Mohammed Al Balushi[3]; [1]Rio Tinto Alcan; [2]Maschinenfabrik Gustav Eirich; [3]Sohar Aluminium

In 2008 a new paste plant comprising an RTA specified Eirich Mixing Cascade EMC was successfully commissioned at Sohar Aluminium. The paper outlines the technological and process developments over the last 15 years leading to this development. The paper starts with the first adaptations of the intensive mixer for use in anode paste mixing, the euipment optimisation to improve paste quality via both laboratory scale trials and small scale industrial trials, the resulting development of the Eirich Mixing Cascade and its initial industrial implementation. Next an overview of the start-up and operations of the Sohar installation is given. This installation consists of two continuous intensive mixers in series producing at rates of up to 36 tonnes per hour. Anode process and quality results from the start up and resulting operation are presented.Finally the paper discusses the further potential development of this type of mixing line.

9:25 AM

New Design of Process Area Based on Math Modelling and Simulation for Buss Kneader Principle in the Application of Green Anode Paste Preparation: *Hans-Ulrich Siegenthaler*[1]; Joel Stampfli[1]; [1]Buss AG

The Buss Kneader principle is known in this application for nearly 60 years. A great development step forward could be achieved recently, when all specific process requirements have been analysed with math modelling and simulation. Based on the results the kneader was redesigned allowing a much more intense mixing process with a micro distribution of the pitch. This paper presents the way to the latest state of the developments to mix green anode paste with specific focus on high anode density combined with high production capacities to achieve the processing and economic advantages as requested by the anode producers today and tomorrow.

9:50 AM

Aluchemie Back to Benchmark: *Patrick Claudel*[1]; Erwin Smits[1]; [1]Aluchemie / Rio Tinto Alcan

Aluchemie was considered in the 90's to be the benchmark in Anodes but made the wrong strategic choices early 2000 and suffered several customer complaints. A new and rigorous approach in 2007 brought us back as the supplier of choice. Our purpose is to share with our peers the success factors and findings of this first step of our journey for a more efficient anode. The team has first drawn Alchemies' *variation finger print*. This tool clearly identifies priorities and develops low effort solutions very quickly. Encouraged by customer feed back and challenged by the results of the variation analysis, the operational teams created a set of basics rules in order to eliminate the worst practices. Finally, Aluchemie established an early warning system to sustain and further improve the level of quality. These 3 elements will be reviewed in detail, illustrated by practical applications and documented findings.

10:15 AM Break

10:30 AM

Successful Start up of the Combined Rhodax® and IMC® Processes at the Sohar Smelter: André Pinoncely[1]; Jean Bigot[2]; Christophe Bouche[3]; [1]Solios Carbone; [2]Rio Tinto Alcan; [3]Fives Solios

In December 2005, Sohar Aluminium Company (Sultanate of Oman) awarded Solios Carbone the turn-key supply of its Green Anode Plant. Upon the successes of the Rhodax® process start up at the Alba line 5, and of the Intensive Mixing Cascade (IMC®) Chinese references, the Sohar anode plant specified by Aluminium Pechiney Technology was the first opportunity to combine these two breaking through technologies. The first anode was produced in March 2008 and the plant performs today beyond expectations at 36 tph capacity. This paper describes the main features and performance of this new plant and highlights the optimizations which resulted from a close collaboration between all parties. Finally it gives some preview of the 60 tph Green Anode Plant presently under commissioning at the Qatalum smelter in Qatar, becoming soon the next reference of such combined process evolution toward the high capacity requirement of modern smelters.

10:55 AM

Amelios™, A Performance Analysis Tool for Green Anode Plant: Christophe Bouche[1]; Oussama Cherif Idrissi El Ganouni[2]; André Molin[1]; [1]Solios Carbone; [2]Fives

Stable anode density is crucial to operate reduction cells at peak performance. AMELIOS is a performance analysis tool combining process expertise, mass balance calculation and data mining, developed to improve green anode density stability and plant productivity. It allows quick identification of process deviation root causes to implement corrective actions. Process parameter time series from PLCs are analyzed in real-time to generate reconciled and synchronized anode process data along with KPI allowing an individual anode tracking throughout the process. A statistical analysis of the anode densities identifies the most influent process parameters. The plant breakdown root causes are analyzed to identify the bottlenecks. This information is made available to maintenance, operators and management to improve process transparency and help them to focus on critical equipment, critical process parameters and plant performance objective. A beta version of AMELIOS™ has been in operation in a Green Anode Plant since April 2009.

11:20 AM

Anode Paste Plants: Innovative Solution for Optimum Emission Performances: *Hugues Vendette*[1]; [1]Solios Environnement Inc.

Coal tar pitch volatiles (PAHs) emitted during paste mixing and anode forming are traditionally captured via coke dry-scrubbers. In recent years, regenerative thermal oxidizers (RTO) have occasionally been used to reduce the emissions of the PAH lighter fractions. However RTOs have relatively high operating costs and can be subject to plugging and fire hazards due to the building-up of condensed tars. This paper presents a new treatment approach that has recently been implemented in new anode plants where dual treatment systems relying on the use of conventional dry-scrubbers and RTOs were supplied. Low PAH concentration streams from the anode former area are treated using a coke dry-scrubber whereas the higher concentration streams from the paste cooler are treated with the combined action of a coke dry-scrubber followed by a RTO. The combination of these two approaches provides the Owner with high capture/destruction efficiency, lower operating costs and very high reliability.

General Abstracts: Light Metals Division: Session I

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee, TMS: Magnesium Committee, TMS: Recycling and Environmental Technologies Committee, TMS: Energy Committee, TMS: Aluminum Processing Committee

Program Organizers: Alan Luo, General Motors Corporation; Eric Nyberg, Pacific Northwest National Laboratory

Wednesday AM Room: 607
February 17, 2010 Location: Washington State Convention Center

Session Chair: Alan Luo, General Motors Research & Development Center

8:30 AM

Alcoa Alumina Refinery Secures Future through Reliability Excellence Efforts: *John Kalpoe*[1]; Keith Johnson[2]; [1]Suralco Alumina Refinery; [2]Life Cycle Engineering

In 2009 alumina prices plummeted, stock values dropped, the price of raw materials rose, and the partnership between Alcoa and BHP was coming to an end, leaving Alcoa Suralco leadership with some very tough business decisions to make. The refinery manager stated that the implementation of Reliability Excellence (ReX) was the foundation of their survival plan. It was this management commitment during the toughest of times that has paid off for Suralco. This paper will cover Suralco's Reliability Excellence journey. The major points will be centered on early challenges, processes, strategy, communication and results. It will show how leadership's commitment, perseverance, and good judgment resulted in a much larger return on investment than expected during a crisis period. This paper will show what Suralco has accomplished in a very tough environment, and how ReX has given them the tools to set a benchmark in their industry.

8:50 AM
Application of ECAP on Commercial Purity Aluminum: *Nilufer Evcimen*[1]; Yahya Bayrak[1]; Ahmet Ekerim[1]; [1]Yildiz Technical University

The present study includes determination and optimization of parameters which were effective on achieving sub-micron grain size on commercial purity aluminum to be able to use for industrial processes. Equal Channel Angular Pressing (ECAP)-Conform process was attempted at room temperature on commercial purity aluminum wire samples. Before ECAP process, heat treatments were applied between 320-450\176C for up to 8 h to remove wire texture. Number of passes was increased systematically. For characterization purposes, optical microscope, scanning electron microscope, SEM and transmission electron microscope, TEM were used. Transmission electron microscopy revealed that sub-micron grain size was attained after 11 passes. Mechanical tests such as hardness and tensile test were conducted to characterize the mechanical properties.

9:10 AM
Assessment of Casting Filling by Modelling Surface Entrainment Events Using CFD: *Mark Jolly*[1]; Carl Reilly[1]; Nick Green[1]; [1]University of Birmingham

The reliability of cast components is dependent on the quality of the casting process. During this highly transient filling phase the prevention of free surface turbulence and consequential oxide entrainment is critical to assure the mechanical integrity of the component. Past research has highlighted a number of events that lead to entrainment of surface oxides. FLOW-3D, flow structures that result in surface entrainment events have been simulated and an algorithm developed that allows entrainment and defect motion to be tracked. This enables prediction of the quantity and motion of oxide film generated from each event. The algorithm was tested experimentally using real-time X-ray radiography and real metal flows. A quantitative criterion is proposed to assess the damage of each type of event. Complete running systems have also been studied to understand how they could be assessed for quality of filling based on the flows within them.

9:30 AM
Behavior of MgO during Forming and Leaching Process of Calcium Aluminate Slag: *Wang Bo*[1]; Sun Huilan[1]; Bi Shiwen[2]; [1]Hebei University of Science and Technology; [2]Northeastern University

MgO is one of the major impurities in calcium aluminate slag. The existence of MgO will decrease the alumina leaching property of calcium aluminate obviously. The effect of MgO on phase components, crystal structure and alumina leaching property of calcium aluminate slag are studied in this paper by the methods of XRD, EDS and SEM. The results indicate that MgO will be dissolved in $12CaO•7Al_2O_3$ crystal and it causes the expansion of crystal cellular and the increasement of interplanar spacing when the content of MgO is lower than 1%. MgO has little effect on alumina leaching ratio of slag under this condition. When the content of MgO is higher than 1%, the compound $20CaO•13Al_2O_3•3MgO•3SiO_2$ which is difficult to leach is formed and decreases the alumina leaching property of calcium aluminate obviously. After alumina leaching process, the major phase of MgO in red mud is $Mg(OH)_2$.

9:50 AM
Effect of Variables on Deposit Characteristics of Aluminum from EMIC-$AlCl_3$ Ionic Liquid Electrolytes: *Debabrata Pradhan*[1]; Ramana Reddy[1]; [1]The University of Alabama

Aluminum alloys were electrorefined from 1-Ethyl-3-methyl-imidazolium chloride (EMIC)-$AlCl_3$ (60 wt%) ionic liquid electrolyte on copper/aluminum cathodes at 90 ± 3°C. The experiments were carried out to investigate the effect of electrode surface masking, anode and cathode materials, surface roughness of electrodes and deposition time on deposit morphology of aluminum and cathode current density. The deposits were characterized using scanning electron microscope (SEM), energy dispersive spectroscopy (EDS) and X-ray diffraction (XRD). It was shown that electrode masking plays an important role on deposition characteristics of aluminum rather than other variables. Electrode masking produced non-dendritic deposit even after 25 hours of experiments. Pure aluminum (>99%) was deposited for all experiments with current efficiency of 91-99%.

10:10 AM Break

10:30 AM
Effects of Microstructure on Fatigue Crack Growth Behavior of 6061-T6 Wrought Alloys: *Anastasios Gavras*[1]; Brendan Chenelle[1]; Diana Lados[1]; [1]Worcester Polytechnic Institute

Fatigue crack propagation of long and small cracks was investigated in wrought 6061-T6 alloys with various grain morphologies. The grain structure was varied using combinations of chemistry, forming, and heat treatment. Low residual stress was ensured during processing to shed light on microstructural effects on crack growth. To evaluate the long and small crack growth behavior of the alloys, compact tension and surface flaw tension specimens were tested at room temperature and constant stress ratio, R=0.1. Microstructure related mechanisms were used to explain the fatigue crack growth behavior at different growth stages. The differences in the near-threshold behavior between long and small cracks were evaluated for each alloy, assessing closure and microstructurally small crack growth effects. Methods for combined closure/microstructure compensation on long crack growth data are provided together with recommendations for their integration in design.

10:50 AM
Electrochemical Characterization of the Al-Mg Foamed Materials in NaCl Solutions: *S. Valdez*[1]; S. Casolco[2]; H. Castañeda[3]; [1]UNAM-ICF; [2]ITESM-Puebla; [3]Battelle Memorial Institute

The AlMg-alloy was made by melting Al and Mg ingot pieces in an alumine crucible, kept in a resistance electrical furnace. The molten alloy was poured into steel containers with NaCl crystals, in order to produce the foamed material. After solidification the salt was removed using hot water. The corrosion resistance properties of the material are characterized by electrochemical techniques. The potentiodynamic polarization and electrochemical impedance spectroscopy were used to elucidate the interfacial mechanisms of the alloy when exposed to 3.5% NaCl (reagent grade) at room temperature. The evolution of dissolution under different exposure conditions was used to characterized the corrosion rate in corrosive environment.Key words: Al-Mg alloys, electrochemical characterization, metallic foams.

11:10 AM
Effect of Variables on Deposit Characteristics of Aluminum from EMIC-$AlCl_3$ Ionic Liquid Electrolytes: *Debabrata Pradhan*[1]; Ramana Reddy[1]; [1]The University of Alabama

Aluminum alloys were electrorefined from 1-Ethyl-3-methyl-imidazolium chloride (EMIC)-$AlCl_3$ (60 wt%) ionic liquid electrolyte on copper/aluminum cathodes at 90 ± 3°C. The experiments were carried out to investigate the effect of electrode surface masking, anode and cathode materials, surface roughness of electrodes and deposition time on deposit morphology of aluminum and cathode current density. The deposits were characterized using scanning electron microscope (SEM), energy dispersive spectroscopy (EDS) and X-ray diffraction (XRD). It was shown that electrode masking plays an important role on deposition characteristics of aluminum rather than other variables. Electrode masking produced non-dendritic deposit even after 25 hours of experiments. Pure aluminum (>99%) was deposited for all experiments with current efficiency of 91-99%.

11:30 AM
Effects of Volume Percent and Aspect Ratio of Short Carbon Fiber on Mechanical Properties of Reinforced Aluminum Matrix Composites: *Yan Pengfei*[1]; Yao Guangchun[1]; Shi Jianchao[1]; Mu Yongliang[1]; [1]School of Materials & Metallurgy, Northeastern University

Carbon fiber reinforced aluminum matrix composites have been prepared by stir casting. Al–4 wt%Cu was selected as a matrix. The samples were prepared with four volume fractions (2, 4, 6 and 8) and three aspect ratios (300, 500, and 700). Then the aging treatment was carried out. A tensile test was performed to evaluate the tensile strength of the composites. The results show that when the content of carbon fibers is 6 vol% the tensile strength of composites increases by 78% and 36% after aging treatment. Hardness test shows that the hardness of the composites increases by 194% and 34%. Moreover, the fracture behavior and crack deflection of composites were investigated using scanning electron microscopy (SEM). The study also shows that the strengthening mechanism depends strongly on fiber volume fraction, aspect ratio and the degree of wetting between fiber and matrix.

11:50 AM
Effective Capital Management – A Case Study: Joe Petrolito[1]; *Martin Richard*[2]; [1]Hatch; [2]Alcoa

Since 2001, Alcoa's Canada Primary Products division and Hatch Ltd have partnered to supply full EPCM services for their Northeast Region. The region includes three smelters in Quebec , two smelters in the Massena region and one in Iceland. This partnership has resulted in significant improvements in the area of capital allocation and cash flow management. Considerable effort is placed on project readiness to ensure proper forecasting in the interest of avoiding reserving capital and the ensuing opportunity loss. By measuring KPI's such as Project Safety, Cost, Schedule and Technical Performance of completed projects across the region, lessons learned/best practices are easily shared. This relationship has proven particularly beneficial to Alcoa during the present period of low LME markets where flexibility of resources and active project portfolio management has been paramount. The management principles adhered to have helped Alcoa to better control/allocate the reduced amount of available capital.

General Abstracts: Materials Processing and Manufacturing Division: Microstructure, Characterization, and Modeling

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS/ASM: Computational Materials Science and Engineering Committee, TMS: Global Innovations Committee, TMS: Nanomechanical Materials Behavior Committee, TMS/ASM: Phase Transformations Committee, TMS: Powder Materials Committee, TMS: Process Technology and Modeling Committee, TMS: Shaping and Forming Committee, TMS: Solidification Committee, TMS: Surface Engineering Committee
Program Organizers: Thomas Bieler, Michigan State University; Corbett Battaile, Sandia National Laboratories

Wednesday AM Room: 601
February 17, 2010 Location: Washington State Convention Center

Session Chair: To Be Announced

8:30 AM
Improving Creep Properties through Grain Boundary Engineering: *Milo Kral*[1]; Daniel Drabble[1]; [1]University of Canterbury

Grain boundary engineering is a promising methodology to improve the properties of many FCC metals and alloys. The aim of the present work was to investigate the feasibility of using grain boundary engineering to improve the high-temperature properties of an austenitic nickel-iron-chromium alloy. Samples of 800H (32%Ni-21%Cr-44%Fe with Al, Ti additions) were 'grain boundary engineered' using a range strain/anneal conditions and then characterized using Electron Backscatter Diffraction (EBSD) analysis. The various processing conditions provided samples with a range of grain size, grain boundary character and grain boundary connectivity. This work has culminated in correlations between the microstructural characteristics and high-temperature material properties such as steady-state creep rate and strength/ductility under typical service conditions.

9:10 AM
Modeling the Anisotropic Properties of Tantalum Taylor Impact Specimens: *Michael Nixon*[1]; Joel House[1]; Brian Plunkett[1]; Joel Stewart[1]; [1]USAF AFRL

Numerical simulations of the Taylor Impact experiment using commercially pure tantalum were performed with isotropic and anisotropic yield surface descriptions of the mechanical properties within the Elastic-Plastic Impact Code (EPIC version 2006). The anisotropic yield surface representation with strain hardening was based upon calculations using the Visco-Plastic Self Consistent model developed by Tome and Lebensohn. The simulation of the high strain rate plastic deformation assuming different yield surfaces allows the comparison of the specimen profile geometry to reveal the effects of anisotropy on the mechanical properties under dynamic loading. The numerical simulations were compared to experimental data from a lot of tantalum with a processing history that included Equal Channel Angular Pressing, forging and annealing. Details of the thermo-mechanical processing and the Taylor Impact experiments are reported by House et al (2010).

9:30 AM
Neural Networks Modeling of Mechanical Properties in Medium Carbon Steels: *N. S. Reddy*[1]; Jae Sang Lee[1]; Yang Mo Koo[1]; [1]GIFT, POSTECH, Pohang, Korea

Neural network (NN) model has been developed for the analysis of the correlation between the mechanical properties and composition and heat treatment parameters of low alloy steels. The input parameters of the model consist of alloy compositions and heat treatment parameters. The outputs of the NN model are mechancial properties. The model can be used to calculate the properties of low alloy steels as a function of alloy composition and heat treatment variables. The individual and the combined influence of inputs on properties of medium carbon steels is simulated using sensitvity analysis. The current study achieved a good performance of the NN model, and the results are in agreement with experimental knowledge. Explanation of the calculated results from the metallurgical point of view is attempted. The developed model can be used as a guide for further alloy development.

9:50 AM
Mathematical Modelling of an Annealing Furnace for Process Control Applications: *Nick Depree*[1]; James Sneyd[1]; S. Taylor[1]; Mark Taylor[1]; M. O'Connor[2]; John Chen[1]; [1]University of Auckland; [2]New Zealand Steel Ltd.

Dynamic thermal models of a continuous annealing furnace have been developed, with the intention of optimising furnace control in both steady state and changing furnace conditions. The models calculate both strip and furnace temperatures, and strip microstructural changes for all operating conditions. Existing manual control during transient operation results in large amounts of strip receiving incorrect heat treatment and products that do not meet specifications. A 3D finite element model has been constructed which is accurate but computationally expensive, and is used to provide understanding of furnace radiative heat transfer and temperature distribution. A reduced dimensionality model from heat transfer fundamentals with a coupled steel recrystallisation model gives rapid results that can be used to optimise steady state settings or simulate the furnace response during transient conditions. Successful furnace optimisation will provide significant financial and energy savings due to reduced wastage and rework of incorrectly heat treated product.

10:10 AM Break

10:30 AM
Dynamic Abnormal Grain Growth in Alpha Iron: *Phi Thanh*[1]; George Kaschner[2]; J.P. Delplanque[1]; Joanna Groza[1]; [1]UC Davis; [2]Los Alamos National Labs

We investigated dynamic abnormal grain growth (DAGG) in alpha iron in attempt to create centimeter-size grains. We performed strain controlled tensile deformation in the temperature range (TH = 0.4 – 0.6) and strain-rates (10-7 to 10-3 s-1). Both constant strain-rate and strain-rate jump experiments were performed to induce DAGG. Once abnormally large grains appear, grain boundary mobility is sustained by balancing dislocation generation and annihilation rate by varying strain-rate at temperature.

10:50 AM
A Study on the Behavior of Boron in Low Carbon Steel by Neutron Autoradiography: *Dong Jun Mun*[1]; Kyung Chul Cho[1]; Eun Joo Shin[2]; Jae Sang Lee[1]; Yang Mo Koo[1]; [1]Pohang University; [2]Korea Atomic Energy Research Institute

It is well known that when trace boron is added to steel, their properties can be considerably improved. It has been shown that the beneficial effect of boron is caused by the segregation of boron at austenite grain boundaries. The distribution behavior of boron in steel such as segregation along the grain boundary and formation of borocarbides or boronitrides is sensitively subject to cooling rate, heat treating temperature, and alloying elements. However, in general, it is well known that a very small amount of boron in steel is hard to be detected with electron spectroscopy because of its low atomic value, so that a special technique is necessary to observe boron distribution in steel. In this present study, the segregation and precipitation behavior of boron in austenite phase was mainly studied by means of Neutron Autoradiography method. From those results, the behavior of boron in low carbon steel was discussed.

11:10 AM

Flexure Strength and Hydrothermal Degradation of 3mol% Yttria-Stabilized Zirconia (3Y-TZP): Microwave vs. Conventional Sintering: *Kirk Wheeler*[1]; Pedro Peralta[1]; Scott Atkin[2]; [1]Arizona State University; [2]Creative Dental Laboratories

Flexure strength was determined for 3Y-TZP samples sintered in either a microwave or a conventional furnace. Microwaved samples showed an increase in flexure strength (~1490 MPa) compared to samples sintered conventionally (~1380 MPa). This was attributed to a nearly 50% reduction in grain size from ~1.0 µm for conventional samples to ~ 0.5 µm for microwave samples, as determined via scanning electron microscopy (SEM). In addition, an accelerated ageing test was performed to simulate the degradation of 3Y-TZP in a humid environment. Samples were tested in a steam environment at ~125 °C and ~200 kPa pressure for 75 hrs. A reduction of flexure strength by ~43% was found for conventionally sintered samples while only a ~14% reduction was measured for the microwaved samples. The increased degradation of the conventionally sintered samples can be attributed to an increase in the monoclinic phase as determined by powder x-ray diffraction.

11:30 AM

Novel Pathways to Hydrogen Dissociation and Diffusion on Pd Alloys: *Heather L. Tierney*[1]; Ashleigh E. Baber[1]; John R. Kitchin[2]; E. Charles H. Sykes[1]; [1]Tufts University; [2]Carnegie Mellon University

This combined scanning tunneling microscopy (STM) and density functional theory (DFT) study shows that individual Pd atoms in an inert Cu matrix are active for the dissociation of hydrogen and subsequent spillover onto Cu sites. The atomic-scale compositions of both Pd/Cu{111} and Pd/Au{111} near-surface alloys were elucidated and H uptake was quantified. Experimental and theoretical results indicated that H spillover was facile on Pd/Cu at 400 K but that the hydrogen diffusion barrier is insurmountable on a Pd/Au sample with the same atomic composition and geometry. These results demonstrate the powerful influence an inert substrate has on the catalytic activity of Pd atoms supported in its surface. While these experiments were performed in ultra-high vacuum, an understanding of the nature of H_2-surface interactions, including molecular adsorption, dissociation and surface diffusion provides a basis for the development of next-generation energy technologies.

11:50 AM

An Investigation on the Flow Behavior of Metals when Forging Specimens Having Different Cross Sections: *Bashir Raddad*[1]; [1]University of Alfateh, Mechanical Department

Experiments were carried out to generate data on cold compression of solid copper and aluminum specimens having different cross section shapes (cylindrical, hexagonal, square and rectangular) and height –to-diameter ratios, between flat dies at two degrees of surface condition (dry or lubricated). Different cross section shapes and surface conditions are expected to create different loading characteristics and modes of deformation during this process. Experimental results showed load/displacement/ curves consisted of many stages: the metal begins to overcome the frictional force at the interface in the first stage and the metal begins to flow after reaching the yield point. This stage is characterized by a steep rate of increase of load. In the second stage, the load was less in the lubricated specimens. And this stage showed the different in load due to the different Ho/Do ratio.

General Abstracts: Structural Materials Division: Non-Ferrous Materials

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Alloy Phases Committee, TMS: Biomaterials Committee, TMS: Chemistry and Physics of Materials Committee, TMS/ASM: Composite Materials Committee, TMS/ASM: Corrosion and Environmental Effects Committee, TMS: High Temperature Alloys Committee, TMS/ASM: Mechanical Behavior of Materials Committee, TMS/ASM: Nuclear Materials Committee, TMS: Refractory Metals Committee, TMS: Titanium Committee

Program Organizers: Eric Ott, GE Aviation; Robert Hanrahan, National Nuclear Security Administration; Judith Schneider, Mississippi State University

Wednesday AM Room: 3A
February 17, 2010 Location: Washington State Convention Center

Session Chair: To Be Announced

8:30 AM

A Creep Rupture Time Model for Anisotropic Creep-Damage of Transversely Isotropic Materials: Calvin Stewart[1]; *Ali Gordon*[1]; [1]University of Central Florida

Anisotropic creep-damage modeling has become an increasingly important prediction technique in both the aerospace and industrial gas turbine industries. The introduction of tensorial damage mechanics formulations in modeling tertiary creep behavior has lead to improved predictions of the creep strain that develops due to anisotropic grain structures and the induced anisotropy that occurs with intergranular damage. A number of isotropic creep-damage rupture time prediction models have been developed in literature however; few rupture time prediction models for tensorial anisotropic creep-damage are available. In this paper, a rupture time model for anisotropic creep-damage of transversely isotropic materials is derived. Comparison with the associated isotropic formulation and the Larson-miller parameter show improved creep rupture time prediction.

8:50 AM

Comparison of Deformation Mechanisms for Constant Strain Rate and Creep Testing of a Ni-Based Superalloy: *Hallee Deutchman*[1]; Raymond Unocic[1]; Michael Mills[1]; [1]The Ohio State University

The effect of microstructure, stress, temperature, and strain rate on deformation mechanisms were investigated under creep and constant strain rate conditions on an advanced, polycrystalline Ni-based disk superalloy. A detailed microstructure characterization aimed at measuring the gamma-prime precipitate size, morphology, distribution as well as grain size and degree of grain boundary serration was performed prior to mechanical testing experiments so that the effects of microstructure can be correlated with the deformation response. Constant load creep tests and constant strain rate tests were performed at the same temperature so that the influence of strain rate on deformation substructure can be assessed. Following mechanical testing, a thorough TEM characterization study was done to determine the operative deformation mechanisms. Mechanisms found included microtwinning and isolated faulting of the gamma-prime precipitates. Funding for this work has been provided by AFOSR through the Metals Affordability Initiative (MAI) program.

9:10 AM

A Combinatorial Approach to Investigate Solid Solution Hardening in Ni-Based Systems by Nanoindentation: *Oliver Franke*[1]; Karsten Durst[2]; Mathias Göken[2]; [1]MIT; [2]University of Erlangen

Diffusion couples are used to study the thermodynamics of a wide range of materials. With nanoindentation local mechanical properties in a diffusion zone can be studied with high lateral resolution. The combination of nanoindentation and scanning electron microscopy can be used to investigate solid solution hardening effects of certain alloying elements quickly and efficiently. In this work a study of three alloying elements (Fe, Mo and Ta) in binary Ni-based systems and Ni-NiAl was carried out. After annealing the diffusion zone was characterized using arrays of indents and EDX.For Ni-NiAl, a significant modulus change is observed in the beta-NiAl-regime. In Ni-Mo, Ni-Fe and Ni-Ta, the solid solution hardening effect was studied as they show solubility over a wide concentration range and the diffusion zone was wide enough to be accessed by nanoindentation. The obtained results can be described by a slight modification of Labusch's model on solid solution hardening.

9:30 AM
Single-Crystal Solidification of New Co-Al-W Base Superalloys: *Masafumi Tsunekane*[1]; Akane Suzuki[2]; Tresa Pollock[1]; [1]University of Michigan; [2]GE Global Research

Solidification processing of new high-temperature Co-Al-W base single-crystals has been investigated. Single-crystal bars with compositions of Co-9.4Al-10.7W, Co-8.8Al-9.8W-2Ta and Co-7.8Al-7.8W-1.5Ta-4.5Cr were successfully grown with a conventional Bridgman process. Primary dendrite arm spacings in each single-crystal were measured to be about 300 µm. Segregation of constituent elements in the dendritic structure was very limited, compared to nickel-base single-crystals. Partitioning coefficients of each element were calculated to be close to 1 from concentration profiles obtained by EPMA. Polycrystalline starters utilized to initiate single-crystal growth were also investigated to consider the possible effect of back diffusion. Segregation characteristics within the starters were similar to the characteristics of single-crystals. These observations collectively suggest that freckle formation is unlikely to occur during solidification in single-crystals of Co-Al-W base alloys.

9:50 AM Break

10:10 AM
Nucleation of Extension Deformation Twins in α-Ti: *Leyun Wang*[1]; Yiyi Yang[1]; Martin Crimp[1]; Philip Eisenlohr[2]; Darren Mason[3]; Thomas Bieler[1]; [1]Michigan State University; [2]Max-Planck-Institut für Eisenforschung GmbH; [3]Albion College

Activity of two extension twinning systems, {10-12}<-1011>(T1) and {11-21}<-1-126}(T2), is observed in textured polycrystalline α-Ti. The crystallographic direction of hexagonal c-axes was preferentially aligned with the global tensile direction resulting from 4-point bending. Hence, most grains are in a hard orientation with low Schmid factors for basal and prismatic slip. T1 twinning was observed much more frequently than T2 twinning. The statistically significant correlation of the alignment between T1 twins and active prismatic slip systems, or, alternatively, other T1 twins, in neighboring grains indicates that nucleation of these twins follows from strain compatibility constraints at grain boundaries. Formation of T2 twins is found to require not only high Schmid factors, but is additionally limited to conglomerates of hard-oriented grains. This preferential activation in hard clusters will be discussed. Support was provided by NSF grant DMR-0710570 and DFG grant EI 681/2-1.

10:30 AM
Influence of Grain Boundary Sliding on Diffusion in Yttria Stabilized Tetragonal Zirconia: *Santonu Ghosh*[1]; Sathya Swaroop[2]; Peter Fielitz[3]; Guenter Borchardt[3]; Atul Chokshi[1]; [1]Indian Institute of Science; [2]VIT University; [3]Technische Universitat, Clausthal

Although there have been suggestions of an enhancement in diffusion because of grain boundary sliding, there are no data available to critically evaluate this possibility. High temperature deformation in a superplastic yttria stabilized tetragonal (YTZ) occurs by grain boundary sliding. In the present study creep experiments were conducted on a fine grained 3 mol% yttria stabilized tetragonal zirconia, under conditions associated with superplasticity at 1598 and 1623K. Grain boundary sliding measurements revealed that the grain boundary sliding contribution to the total creep deformation is >75%. Tracer diffusion studies under creep conditions and without load indicate that there is no enhancement in either the lattice or grain boundary diffusivities. The experimental creep data are consistent with an interface controlled diffusion creep model.

10:50 AM
Constitutive Response of Polymers, Filled and Unfilled, as a Function of Temperature and Strain-Rate: *Eric Brown*[1]; Carl Cady[1]; George Gray III[1]; Mathew Lewis[1]; Dana Dattelbaum[1]; [1]Los Alamos National Laboratory

Recently, interest has been shown concerning the mechanical response of polymers and polymer composites for several reasons. First, evidence has shown that there may be issues with aging and nitroplasticizer uptake. The second area of focus was related to the development of predictive materials models that describe the mechanical behavior of these materials. Accordingly, detailed information about the constitutive response is crucial. Compression measurements were conducted on these materials as a function of temperature from -55°C to +70°C and strain rate using a specially-designed split Hopkinson pressure bar (strain rate of ˜ 2800 s^{-1}) and quasi-statically (strain rates from ≈ 0.001 to 1 s^{-1}) using a hydraulic load frame. The mechanical response of the filled VCE showed a strong dependency on strain rate and was most sensitive to changes in test conditions. The filled foam materials were much less sensitive to changes in temperature or strain rate. The visco-elastic recovery of VCE is seen to dominate the mechanical behavior at temperatures above the glass transition temperature (T_g). It also exhibited increasing elastic loading moduli, E, with increasing strain rate or decreasing temperature, which is similar to other polymeric materials and there is a pronounced shift in the apparent T_g to higher temperatures as the strain rate is increased. Analysis of the filled materials implies damage in the filler material as indicated by a load drop on the stress-strain curve.

11:10 AM
Shape Memory Behavior of an Ultra-Fine Grained Ti-30Ni-20Pd Alloy through Equal Channel Angular Extrusion (ECAE) Processing: *Rabindra Mahapatra*[1]; Charles Lei[1]; [1]Naval Air Systems Command

The Ti-30Ni-20Pd Alloy (in at.%) was ECAE processed to produce ultr-fine grains of 0.5-1 micro-meter. The effects of ultra-fine grain and alloying with Pd on transition temperature and fracture toughness of the alloy relative to Ni-Ti binary alloy will be presented. The effects of phase transformation and related microstructure on transition temperature behavior of the alloy will be dicussed.

11:30 AM
High Temperature Creep-Fatigue Crack Growth Models: *Jeffrey Evans*[1]; [1]University of Alabama in Huntsville

There are numerous applications in the modern engineering world which involve the use of metals under conditions of cyclic loading in operating conditions that can cause creep and/or environmental interactions with time independent, mechanical fatigue processes. Various approaches for modeling the creep-fatigue crack growth behavior have been proposed to capture the various types of damage that is occurring. These include mechanistic modeling, crack growth modeling using the method of superposition to incorporate time-dependent and cycle-dependent components, and numerical modeling. A number of phenomena have been investigated to obtain a better understanding of the fundamental creep-fatigue crack growth process. The various models and techniques used in modeling the elevated temperature creep-fatigue crack growth process will be reviewed.

Global Innovations in Manufacturing of Aerospace Materials: The 11th MPMD Global Innovations Symposium: Innovations in Primary and Secondary Forming - Nickel

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Shaping and Forming Committee, TMS: High Temperature Alloys Committee
Program Organizers: Deborah Whitis, General Electric Company; Thomas Bieler, Michigan State University; Michael Miles, BYU

Wednesday AM February 17, 2010 — Room: 306 — Location: Washington State Convention Center

Session Chairs: Dan Sanders, Boeing Corporation; Lee Semiatin, AFRL-RX

8:30 AM Invited
Technical and Manufacturing Innovations Required to Meet Global Aerospace Requirements for the 21st Century: *Anthony Banik*[1]; [1]ATI Allvac/Allegheny Technologies

The metals industry has reached the 10% mark of the 21st Century. The demand for aerospace materials reached an initial peak at the start of the century spurring a considerable investment in product and process development to meet the demands of this expanding market. Allegheny Technologies is stepping up to this challenge by making substantial investments through a combination of new materials development, advanced modeling capabilities, expanded data acquisition systems, as well as substantial investments in infrastructure. Based on information from the beginning of the century, the expectations for the 21st century will be considered in light of the current performance. As a result, the focus for the next steps in the development, melting and conversion of aerospace materials will be discussed from a producer's perspective in meeting the aerospace market demands for higher temperature, extended life and highest value to aircraft OEMs.

9:00 AM Invited
Some Challenges in Current and Future Superalloy Production: *Lesh Patel*[1]; [1]Special Metals Corp

Nickel Superalloys continue to be the alloys of choice for critical components in a range of industries from Aerospace to traditional and emerging Energy Production systems. Along with the classic challenges of developing alloys which will meet the property requirements of these demanding new applications, materials manufacturers are wrestling with the need for bigger and bigger components in these new systems. This requires different thinking and sometimes new approaches to melting and processing these alloys in order to avoid segregation and other melt related defects in large ingots and also forging and other downstream hot working difficulties. This paper gives some examples and a perspective on these issues.

9:30 AM
Accelerating Insertion of Materials at GE Aviation: Deborah Whitis[1]; *Arturo Acosta*[1]; Shesh Srivatsa[1]; Daniel Wei[1]; [1]General Electric Company

Material and process development for aircraft engines has, in the past, required long and costly experimental programs, imposing a significant barrier to the insertion and exploitation of new materials and manufacturing processes. With the advent of computer modeling and simulation of materials processing, and the accelerated insertion of materials (AIM) approach, we have begun to provide the tools to industrial materials designers that they need to increase productivity and reduce cost of alloy and process development. This presentation will provide an overview of the implementation of the AIM approach at GE Aviation. The integration of materials models, historical databases, and analysis tools have allowed us to more rapidly downselect new alloys and manufacturing processes, responding quickly to the design requirements of a particular component and engine environment. Current progress in applying these techniques to nickel-based superalloys will be reviewed.

9:50 AM
Constitutive Model of Superplastic and Power-Law Creep Deformation during Isothermal Forging of P/M Alloy René 88DT: *Wen Tu*[1]; Tresa Pollock[1]; [1]University of Michigan

Deformation mechanisms during isothermal compression of P/M alloy René 88DT has been studied. Grain level analysis by electron backscatter diffraction is used to quantify different microstructural phenomena that occur during both superplastic and power-law creep deformation. A constitutive model including all straining mechanisms and concurrent microstructural phenomena has been created to predict the grain structure evolution during isothermal compression. During superplastic deformation at lower strain rates, excess vacancies created at the grain boundaries increase grain boundary mobility causing enhanced grain growth. The quantity of excess vacancy created follows an Avrami solution as a function of temperature and strain rate. During power-law creep deformation at higher strain rates, dynamic recrystallization initiates after a critical local stored deformation. This critical stored energy for dynamic crystallization is measured experimentally as a function of strain rate. Experimental results for grain size are compared to those predicted by the grain structure evolution model.

10:10 AM Break

10:30 AM
$\gamma - \gamma' - \delta$ Ternary Eutectic Ni-Base Superalloys Alloys Amenable for Manufacture: Yijing Shi[1]; Alejandro Rodriguez[1]; Mengtao Xie[1]; Randy Helmink[2]; Mark Hardy[3]; *Sammy Tin*[1]; [1]Illinois Institute of Technology; [2]Rolls-Royce Corporation; [3]Rolls Royce plc

As one of the most important classes of high-temperature structural materials, Ni-base superalloys are critical to the continued development of high-performance turbine engines for propulsion and power generation. In order to accommodate the increases in engine operating temperatures required for improved performance and efficiency, higher concentrations of refractory alloying elements have been used to enhance the mechanical properties of Ni-base superalloys. However, many of these compositional modifications have also tended to result in the alloy being more difficult to manufacture into large-scale components using traditional approaches and techniques. The present investigation evaluates the novel Ni-Nb-Cr-Al alloys, based on the pseudo-ternary eutectic $\gamma - \gamma' - \delta$ system, that exhibit promising physical and mechanical properties for turbine engine applications.

10:50 AM
Microstructure and Properties of Platinum-Group-Metal Modified Nickel-Base Superalloys: *Adam Pilchak*[1]; Donald Weaver[2]; Donna Ballard[2]; S. Semiatin[2]; [1]Universal Technology Corporation; [2]Air Force Research Laboratory

The addition of platinum-group metals (PGM) to nickel-base superalloys can significantly enhance their oxidation resistance. Thus, these alloys are being developed as candidate materials for metallic thermal protection systems for use at high temperature. In the present work, the microstructure and properties of wrought PGM-modified superalloys were investigated and compared to those of commercially-produced alloys such as Haynes® 230. For this purpose, cast ingots were forged or extruded and subsequently hot-pack rolled to produce sheet and foil. The resulting microstructures were characterized using scanning electron microscopy and electron backscatter diffraction, and elevated-temperature tensile and compressive strengths were measured.

11:10 AM
Modelling the Effect of Initial Heat-Treatment on the Creep of Multi-Modal Nickel Superalloys: *James Coakley*[1]; Hector Basoalto[2]; David Dye[1]; [1]Imperial College; [2]QinetiQ

Polycrystalline nickel superallyos used in aero-engine disc applications can often possess a bimodal gamma prime microstructure, for example in NI115 and René 80. During heat treatment and service the gamma prime distribution can evolve, with consequent effects on the creep behaviour. Here a modified LSW coarsening model is presented to model the effect of heat treatment and service conditions on the precipitate distribution. The distribution is then used in a physically-based, phenomenological creep model, based on the work of Dyson and McLean, to predict the effect of heat treatment on the creep behaviour. The results are compared to experiment for creep tests and heat treatments performed on NI115.

11:30 AM
Flow Behavior of Superalloy 945 during High Temperature Deformation: *Steve Coryell*[1]; Kip Findley[1]; Martin Mataya[1]; [1]Colorado School of Mines

The demand for improved materials is continuously pushing producers to obtain a fine grain structure and tight restrictions on grain size uniformity in forged superalloy rod. Understanding flow and recrystallization behavior is critical for optimizing forge and annealing practices to meet these requirements. The flow behavior of INCOLOY® alloy 945, a newly developed hybrid of alloys 718 and 925 with a unique combination of strength and corrosion resistance, was performed using uniaxial compression testing at elevated temperatures, characteristic of hot working. Compression was performed at temperatures ranging 950°-1150°C and strain rates ranging 0.001-1.0s^{-1}. Flow and peak stresses increased with strain rate and decreasing temperature, shown by the Zener-Holloman relationship. Material constants such as the activation energy for deformation, stress exponents, and strain rate sensitivities were determined as a prerequisite for developing mathematical models for the constitutive behavior of INCOLOY® 945. Possible mechanisms causing distinct flow characteristics will also be discussed.

11:50 AM
Microstructure Based Monotonic Stress-Strain Modeling of R-104 as a Function of Temperature: *Sujoy Kar*[1]; Sanjay Sondhi[1]; Daniel Wei[2]; David Mourer[2]; [1]GE Global Research; [2]GE Aviation

Nickel based superalloy René 104 is a polycrystalline turbine disk alloy. The stress-strain response of this alloy is dependent on microstructure and the operative damage mechanisms. Deformation mechanisms vary in different temperature regimes and plastic strain levels. The model developed is based on Estrin's dislocation based framework. Equation sets have been adapted to capture different in-elastic hardening and softening mechanisms operative at different temperature regimes for René 104. In the present paper, the details of the monotonic stress-strain model and its predictive capability on different microstructures and at different temperatures will be described.

12:10 PM
Effects of Temperature, Deformation Strain, and Slow Transfer on the Microstructure and Mechanical Properties of 304L Stainless Steel Forgings: *Nathan Switzner*[1]; Robert Bergen[2]; Jamie McQueen[1]; James Knutson[1]; [1]Honeywell FM&T; [2]Precision Metal Products, Inc

304L forgings were made in a High Energy Rate Forging (HERF) press at hot working temperatures of 1550°F and 1725°F. Prior to forging, the preform shape had a "mountain" appearance in the side view, with the intent of gathering information about multiple strain levels from a single sample. We also varied the time of transfer between heating furnace, forging press, and water quench. Mechanical testing and microstructural analysis were conducted on final forgings. Intuitively, room temperature yield and ultimate strength increased with deformation strain; however the high deformation strain levels of approximately 1.5 to 2.0 EQPS resulted in decreased strength due to deformation heating. Added transfer time resulted in a slight increase in strength; but at the higher strain levels, deformation softening eliminated the effects of delayed transfer. The deformation process was modeled with ABAQUS coupled thermal-mechanical simulation to predict final shape and properties.

Hume-Rothery Symposium: Configurational Thermodynamics of Materials: Session V

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Chemistry and Physics of Materials Committee
Program Organizers: Chris Wolverton, Northwestern University; Mark Asta, University of California, Davis; Gerbrand Ceder, Massachusetts Institute of Technology (MIT)

Wednesday AM Room: 212
February 17, 2010 Location: Washington State Convention Center

Session Chair: To Be Announced

8:30 AM Invited
Order-Disorder in the Phase Field Crystal Model: *Jeffrey Hoyt*[1]; Ken Elder[2]; [1]McMaster University; [2]Oakland University

Over the course of his career, Didier de Fontaine has made several significant advances in the study of phase equilibria, thermodynamics and kinetics of ordering in alloys. In this work we use the ideas of de Fontaine to formulate a phase field crystal model (PFC) that can describe the order-disorder phenomenon. It is shown that a simple extension to the original binary alloy PFC free energy leads to a rich variety of phase diagrams. In addition to a liquid and a high temperature disordered phase, the PFC model can stabilize the BCC based ordered phases B2, B32 or DO_3 depending on the choice of a single length scale parameter. Several applications of the model will be discussed including ordering kinetics, the variation of long range order within the vicinity of dislocations and grain boundaries, and disorder trapping during rapid solidification.

9:00 AM Invited
Phase Equilibria, Microstructural Evolution and Coarsening Kinetics In "Inverse" Ni_3Ge (γ')-Ni(Ge) (γ) Alloys: *Alan Ardell*[1]; Yong Ma[2]; [1]National Science Foundation; [2]UCLA

The phase boundary separating the γ' and (γ + γ') regions of the Ni-Ge phase diagram was established from 700 to 1000 °C in alloys containing 22.0 to 23.5 at.% Ge. "Inverse" γ' alloys were aged to study the kinetics of the precipitation of the γ phase. The precipitate shapes change from spherical to large non-equiaxed plates as the size increases; coalescence is responsible. γ precipitates are more strongly spatial correlated than γ' precipitates in normal Ni-Ge alloys and coalesce faster at all volume fractions (f_e). The γ precipitates grow by diffusion-controlled coarsening with a rate constant $k(f_e)$ that increases with increasing volume fraction, f_e. The particle size distributions are broader than the theoretical distribution of the LSW theory in most of the alloys. The kinetics of coarsening of γ precipitates in inverse alloys is much slower than in normal alloys, as expected from chemical diffusion in the two phases.

9:30 AM Invited
Phase Field Crystals: Atomistic Simulations on Diffusive Timescales: Kuo-An Wu[1]; *Peter Voorhees*[1]; [1]Northwestern University

Phase field crystal models have been used to describe a wide range of phenomena from grain growth to solidification. The strength of the method lies in its ability to follow the atomic scale motion that accompanies a process that occurs on diffusive timescales. As illustrations, we discuss the effects of an applied stress on the stability of a solid-liquid interface and the evolution of grains in crystals. The grain growth simulations show the evolution of the dislocation structure of a grain boundary and the local atomic displacements of atoms near the boundary during grain growth. We find that dislocation reactions play an important role in grain morphology and rotation. The simulations of the stress-driven interfacial instability illustrate the importance of the structure of the solid-liquid interface on the evolution of the instability.

10:00 AM Break

10:30 AM Invited
Phase Field Modeling of the Martensitic Transition: Intermittent Dynamics and Self-Organized Criticality: *Alphonse Finel*[1]; Oguz Salman[1]; [1]ONERA

Martensitic transformations in shape memory alloys are characterized by large strain misfits between austenite and martensite. The transitions are often athermal, dominated by elastic accommodation, and the dynamics are essentially thermoelastic. We first present a qualitative picture of the physical mechanisms that lead to thermoelasticity. On a macroscopic scale, partial accommodation with finite polytwinned domains, together with internal constraints, is responsible for the thermoelastic behavior. On a finer scale, due to pinning effects, the thermoelastic dynamics consists in a large series of metastable equilibrium states separated by instabilities. Next, using a lagrangian method that incorporates inertia, we present a quantitative analysis of the cubic-to-tetragonal martensitic transition in a Fe-Pd alloy. We show that the dynamics is critically self-organized: it consists in a large series of bursts that display power-law distributions. Finally, we compare our results with a recent experimental investigation of the acoustic emission observed in a Fe68.8Pd31.2 single crystal.

11:00 AM Invited
Quantitative Phase-Field Simulations of Growth and Coarsening in Polycrystalline Multi-Component and Multi-Phase Materials: *Nele Moelans*[1]; Liesbeth Vanherpe[2]; Jeroen Heulens[1]; Bert Rodiers[3]; Bart Blanpain[1]; Patrick Wollants[1]; [1]K.U. Leuven, dept. Materials Science and Engineering; [2]K.U. Leuven, Dept. Computer Science; [3]LMS International

Phase-field modeling has become very important for simulating microstructure evolution. It has been applied to study solidification, precipitation, grain growth, martensitic transformations and many more phenomena. To account for alloy specific properties --such as phase equilibria, interface energy and kinetics, diffusion coefficients, elastic properties, and crystal structure and orientation relationships--, phase-field models rely on experimental measurements and other modeling techniques (e.g. first principles, CALPHAD and molecular dynamics). With a naive model formulation, however, the relations between model parameters and alloy properties are too complicated so that realistic simulations are practically unfeasible for multi-phase, multi-component or polycrystalline alloys. We discuss state-of-the-art phase-field models that can account accurately for the effect of interface and bulk properties on the evolution of grain morphology and solute distribution at the mesoscale. Attention is given to their applicability to multi-component alloys. The capabilities of the models are illustrated using recent simulation results.

11:30 AM
3D-Microstructures at the Atomic Scale: A Monte Carlo Method with Elastic Interactions: *Varvenne Celine*[1]; Alphonse Finel[1]; Mathieu Fevre[1]; Yann Le Bouar[2]; [1]ONERA; [2]CNRS

It is well-known that size effects have a great influence both in phase diagrams and microstructure morphology. The choice of an atomic scale study is relevant to describe thin interfaces, which is very common in bulk materials, and to reproduce realistic kinetics of precipitation. Furthermore, it allows a direct link between quantitative interatomic potentials and thermodynamics. An efficient way for this study is to combine the lattice static (LS) formalism with Monte Carlo statistical mechanics : the former allows us to treat elasticity in coherent microstructures and the latter to calculate structural and thermodynamic properties. A particular attention has been devoted to the long wavelength limit of the LS and its link with the continuum linear elasticity (as implemented in phase field methods). Moreover, a special effort has been made to have an efficient code, in order to simulate systems large enough to analyse 3D microstructures in ordered binary alloys.

11:50 AM Invited
Effect of Biaxial Strain on Phase Stability and Microstructure Development in Single-Crystal Films: *Long Qing Chen*[1]; [1]Pennsylvania State University

This presentation will discuss the phase transitions and microstructure evolution in thin films. The focus is on the effect of biaxial strains, e.g., from the mechanical constraint by a substrate due to lattice mismatch or thermal mixmatch, on phase and microstructure stability. Two types of phase transitions will be considered, namely, ferroic and isostructural phase separation. It is shown that the shifts in the thermodynamic instability temperatures and the nature of phase transitions can be predicted from purely classical thermodynamic analysis. An efficient, full spectral numerical method will be presented for solving the order parameter and composition evolution equations describing the morphological and microstructural evolution in thin films for which the boundary condition along the out-of-plane direction is non-periodic. It is shown that a biaxial strain can drastically change the relative phase stability, volume fractions of differently orientated domains and the domain-wall orientations, as well as compositional distributions.

Jim Evans Honorary Symposium: Primary and Secondary Production of Metals

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division, TMS Light Metals Division
Program Organizers: Ben Li, University of Michigan; Brian G. Thomas, University of Illinois at Urbana-Champaign; Lifeng Zhang, Missouri University of Science and Technology; Fiona Doyle, University of California, Berkeley; Andrew Campbell, WorleyParsons

Wednesday AM   Room: 620
February 17, 2010   Location: Washington State Convention Center

Session Chair: Lifeng Zhang, Missouri University of Science and Technology

8:30 AM Introductory Comments

8:40 AM
Low Cost $TiCl_4$, the Indispensable Compound to Make Titanium: *James Withers*[1]; J. Laughlin[1]; Y. Elkadi[1]; A. Putilin[1]; R. Loutfy[1]; [1]MER Corporation

Titanium tetrachloride ($TiCl_4$) is indispensable to make pigment (TiO_2) as well as titanium metal by the metallothermic and electrolysis processes. Traditionally ($TiCl_4$) is produced from an ore source as a particulate and carbon in a fluid bed at approximately 1000°C which requires extensive fractionation to purify the $TiCl_4$. An alternate process carbothermically treats the ore as very fine particulate provides ore purification and produces a suboxide-carbide (TiO_xC_y) as an XRD identifiable compound. The TiO_xC_y containing both stoichiometric oxygen and carbon can be chlorinated as low as 180°C – 200°C which produces only $TiCl_4$ in a purified form thus eliminating subsequent fractionation. The lower cost tickle can be used to produce titanium by the standard Kroll process or alternative processing in a re-engineered Kroll process or electrolysis that produces a highly purified powder product. Discussion includes carbothermic reduction, the low temperature $TiCl_4$ synthesis and titanium produced from the $TiCl_4$.

9:05 AM
The Optimization of the Coke and Agglomerate Quantity in Lead Production in "Water-Jacket" Furnace: *Ahmet Haxhiaj*[1]; Egzon Haxhiaj[2]; [1]University of Prishtina; [2]American University in Kosovo

Paper contains the analysis of technological process depending on the composition of lead (Pb) in agglomerate, and the theoretical and real rapport of coke consumption per tone of technical lead produced. The findings are based in the work of "Water-jacket" furnace in Trepça. Paper brings the results of theoretical and experimental studying, along with analytical and graphical analyses of regional thermal balance depending on the composition of load, and the coke quantity in load. While analyzing the technological process of technical lead production we have been searching for the growth of technical lead quantity produced depending on lead percentage in agglomerate and the air that is enclosed in the furnace. Moreover, we aimed to optimize the percentage of lead in agglomerate and the parameters of the process. Simultaneously, keeping the attention to the growth of technical lead produced, the minimization of energy consumption, and the minimization of environment pollution.

9:30 AM
Wireless Instrumentation of Aluminum Smelting Operatings: *Dan Steingart*[1]; James Evans[2]; Paul Wright[2]; [1]City College of New York; [2]Wireless Industrial Technologies

Wireless instrumentation has been demonstrated in locations heretofore unfeasible for measurement within aluminum smelters in demonstration and pilot projects over the past five years. Quantities such as heat flux at the shell, duct exhaust temperature and flow rate, individual anode current and bridge position have been correlated with cell potential. With these sensors we have been able to suggest improved pot maintenance schedules, and also predict anode effects almost 90 seconds before the event occurs. In addition to reviewing the data gathered from these wireless devices, this presentation will touch up methods for powering sensors from environmental sources within power plants.

9:55 AM Break

10:10 AM
The Development of Product Microstructure "Morphology Maps" and their Significance in Describing the Decomposition of Solids: *Peter Hayes*[1]; [1]University of Queensland

The decomposition of solids in reactive gas atmospheres has been the subject of numerous studies over a wide range of chemical systems. Whilst significant advances have been made in understanding and describing the influence of gas phase mass transfer on these processes, the key process phenomena and physico-chemical properties of the solid phases determining the product morphologies have remained less well characterised. These product morphologies can, however, be critical in determining the rate limiting reaction mechanisms and the overall rates of reduction. By considering the fundamental processes occurring at the reaction interface the conditions for the formation of various product morphologies are identified, and the methodology and theoretical basis for the development of morphology maps established. The methodology is shown to be general, and can be applied to the analysis of any system involving the decomposition of metal compounds in reactive gas atmospheres.

10:35 AM
Development and Application of Dynamic Soft Reduction Technology for Continuous Casting Machine: *Cheng Ji*[1]; Miaoyong Zhu[1]; [1]Northeastern University of China

Dynamic soft reduction is an effective method to reduce the central segregation and porosity of continuous casting strands. Based on the review of the previous work, the investigation and development of dynamic soft reduction key technologies, such as soft reduction parameters design, on-line predication of strand solidification end, the dynamic soft reduction control model, and the corresponding process control system, are presented in this paper. The applications in Baosteel Meishan No.2 slab, Panzhihua steel No.2 bloom, and Xingtai steel No. 5 bloom continuous casting machines in China are introduced, and the detail macro structure and center carbon segregation inspection results pre and post the technology application have been demonstrated.

11:00 AM
Transient Behavior of Inclusion Chemistry, Shape and Structure in Fe-Al-Ti-O Melts: Effect of Titanium/Aluminum Ratio: *Cong Wang*[1]; Sridhar Seetharaman[1]; [1]Carnegie Mellon University

The effect of Ti/Al ratio on inclusion behaviors was investigated in aluminum and titanium deoxidized iron melt. When the Ti/Al ratio was maintained at 1/4, titanium-containing oxides exist temporarily after titanium addition, generating little shape change and producing transient stage inclusions with low titanium contents. When the Ti/Al ratio was increased to 1/1, inclusions showed a distinct increase in the titanium content. The transient reaction was accompanied by an irreversible shape change from spherical to irregular. When the Ti/Al ratio in the melt was further increased to 15/1, the inclusion population evolved from spherically-dominant case to irregular ones with the final inclusion chemistry has more titanium. When the Ti/Al ratio in the melt was increased to 75/1, the inclusions evolved towards TiOx inclusions, and this is accompanied by a shape change from spherical to irregular. TEM results confirmed the existence of Ti2O.

Magnesium Technology 2010: Cast Alloys, Casting, and Grain Refinement

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Magnesium Committee
Program Organizers: Sean Agnew, University of Virginia; Eric Nyberg, Pacific Northwest National Laboratory; Wim Sillekens, TNO; Neale Neelameggham, US Magnesium LLC

Wednesday AM — Room: 613
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Mei Li, Ford Motor Company; Norbert Hort, GKSS Research Center

8:30 AM
Effects of Section Thicknesses on Tensile Properties of Permanent Mould Cast Magnesium Alloy AJ62: *Jonathan Burns*[1]; Lihong Han[1]; Henry Hu[1]; Xueyuan Nie[1]; [1]University of Windsor

Applications of high temperature magnesium alloys as structural materials commonly employ high-pressure die-casting processes. Among these magnesium alloys, AJ62 shows great die-castability for automotive engine blocks. However, its potential for use in less expensive, gravity-fed processes that achieve relatively thick sections remains to be demonstrated. Development of such a process will lead to a greater range of applicability for this remarkable alloy. In this study, step-castings of AJ62 were produced in a gravity-fed, permanent mould to understand the mechanical effects of section thickness. Specimens of four varying thicknesses were prepared from respective steps in the castings, and subsequently tested in tension at room temperature. A general degradation of mechanical properties was observed as thickness increased. Evident variations in microstructure for each thickness were also observed via porosity measurements and microstructural analysis. Thereby, an attribution of the changes in mechanical performance to differences in microstructure evolution during solidification can be made.

8:50 AM
Growth Restriction Factor Effects near the Surface of High Pressure Die Cast Mg-Al Binary Alloys: *Anumalasetty Nagasekhar*[1]; Carlos Caceres[1]; Mark Easton[2]; [1]The University of Queensland; [2]Monash University

Solute concentration effects on the grain microstructure at the corner, surface and core regions of the cross-section of high pressure die cast Mg-Al alloys have been evaluated, for Al contents between ~ 6 and 12 mass%, using electron back scattered diffraction technique. The grain microstructure is bimodal in all cases, but especially at the core, due to the prevalence of large dendritic grains formed in the shot sleeve. The average grain size near the surface and at the corner regions is controlled by the amount of solute in the same way as in quiescent castings. Keywords: Magnesium-aluminum alloys,High pressure die casting, Grain size, Growth restriction factor, Electron back scattered diffraction, AZ91 alloy

9:10 AM
Strengthening Mechanisms in Mg-Al-Sn Based Alloys: Shaul Avraham[1]; Alexander Katsman[1]; *Menachem Bamberger*[1]; [1]Technion- Israel Institute of Technology

New creep resistant and microstructurally stable Mg-Al alloys for elevated temperatures are of both scientific and engineering interest. The presence of Al results in the formation of the creep deteriorating γ-$Mg_{17}Al_{12}$ at the grain boundaries (GB). The modification of AM50 with Sn (Base) and Ce (Base+Ce) was investigated by computational thermochemistry (CT), microstructural stability tests and creep tests. Microhardness measurements proved the thermal stability of the alloys during prolonged aging at 200°C. The stress exponent for both alloys is typical of dislocation climb controlled creep at low temperatures (n=7). The $Al_{11}RE_3$ formation at the GB results in reduced GB sliding and enhanced creep resistance. The Mg_2Sn fine densely dispersed precipitates formed in the α-Mg matrix. The enhanced threshold stress is attributed to dislocation-precipitate interaction. The activation energy for creep in the Base+Ce alloy is higher than in the Base alloy and close to the Mg self-diffusion energy.

9:30 AM
Numerical Simulation and Experimental Study of Squeeze Casting Magnesium Alloy AM50: *Zhizhong Sun*[1]; Henry Hu[1]; Alfred Yu[1]; [1]University of Windsor

The heat transfer measurements are rarely performed in squeeze casting. With different applied pressure levels, the heat transfer rate and heat flow patterns becomes more important in squeeze castings. The paper discussed the effect of applied pressures on the solidification and cooling behavior of a cylindrical squeeze casting of magnesium alloy AM50A. Due to high temperature gradient between the molten metal and the steel die, heat flow in boundary layers is affected by partial solidification. The temperature distributions, the cooling curves, the shape and position of the phase front were simulated with the commercial CFD software Flow3D®. The results show that the application of high pressures result in rapid heat transfer across casting/die interface, and consequently increase solidification and cooling rates. To verify prediction, temperature measurements at various locations inside an experimental squeeze casting were performed. Comparisons of the numerical results with the experimental measurements show close agreement.

9:50 AM
Section Thickness and the Skin Effect in a High Pressure Die Cast Mg-12%Al Alloy: *Kun Yang*[1]; Anumalasetty Nagasekhar[1]; Carlos Caceres[1]; [1]The University of Queensland

Microhardness maps of cast-to-shape tensile specimens of rectangular and circular cross-sections have been produced for a range of alloys. In comparison with that at the centre, the hardness is generally higher near the surface and at the corners of the cross-section. The difference is hardness value is accounted for by the coarser solidification microstructure and the concentration of porosity at the casting's core. The evidence indicates the presence of a harder surface layer (or skin) around the periphery of the cross section; however, the harder layer appears patchy, uneven and asymmetrical, questioning the concept of a definable skin which is uniform and continuous in both hardness and depth. Physical reasons for these features of the casting's skin are discussed.

10:10 AM
Investigations on Microstructure and Properties of Mg-Sn-Ca Alloys with 3% Al Additions: Fady Elsayed[1]; Tarek Abuleil[1]; Ahmed Abd El-Aziz[2]; Karl Kainer[1]; *Norbert Hort*[1]; [1]GKSS Forschungszentrum Geesthacht GmbH; [2]Department of Materials Science, German University in Cairo

New magnesium alloys based on the Mg-Sn system have been studied with an emphasis on the Mg-Sn-Ca system due to their attractive property profile. This research work investigates the effect of 3 wt.% Al additions on two selected Mg-Sn-Ca alloys namely the Mg-3Sn-2Ca (TX32) alloy, and the Mg-9Sn-1Ca (TX91) alloy at different temper conditions (F, T4, T6). The aim is to improve room temperature mechanical properties and corrosion resistance. A comparison of experimental results for the new Mg-Sn-Al-Ca (TAX) alloys is performed with their base Mg-Sn-Ca (TX) alloys and explicitly discussed. Al additions were found to have a favourable effect on strength of Mg-Sn-Ca (TX) alloys while they caused rapid decrease in their corrosion resistance. Furthermore the results show a significantly deteriorated corrosion resistance with respect to the addition of Al.

10:30 AM
Simulation of Stresses during Casting of Binary Magnesium-Aluminum Alloys: Matthew Pokorny[1]; Charles Monroe[1]; *Christoph Beckermann*[1]; Z. Zhen[2]; Norbert Hort[2]; [1]University of Iowa; [2]GKSS Research Centre Geesthacht

A viscoplastic deformation model is used to predict thermal stresses and hot tear evolution during casting of binary Mg-Al alloys. The predictions are compared to experiments that allow for the measurement of contraction forces during solidification and cooling. These force measurements, together with estimates from data found in the literature, are used to obtain the high-temperature mechanical properties needed in the deformation model. The coherency and yielding behavior of the semi-solid material during solidification is investigated in detail. The model is then used to predict the hot tears observed in the experiments. The simulation results show good agreement with the measurements. In particular, the hot tear severity is well predicted for a range of alloy compositions and initial mold temperatures.

10:50 AM
Study on the Microstructure Changes during the In Situ Tensile Processes of as-Cast and Aged Specimens of High-Vacuum Die-Cast Mg-9Al-1Zn Alloy: Jie Song[1]; *Shou-Mei Xiong*[1]; [1]Tsinghua University

The microstructure and mechanical properties of the as-cast, solution treated and aged specimens of high-vacuum die-cast Mg-6Al alloy was studied, and the precipitation behavior during the aging procedure was also analyzed by using scanning electron microscopy, vickers micro hardness test, differential scanning calorimetry and transmission electron microscopy observation. The β-Mg17Al12 phase of Mg-6Al alloy dissolved in the matrix from the as-cast stage to the solution stage, and then small β particles precipitated from the grain boundaries of the matrix during the aging process. The specimens were aged for different time periods at three different temperatures for better understanding of the precipitation behaviors. The skin regions were more favorable to the precipitation during the aging process than the center ones. Factors influencing the heat treatment and precipitation processes were discussed.

11:10 AM
Structure-Property Relationships for Die-Cast Magnesium Alloys: *Jeffrey Wood*[1]; J.P. Weiler[1]; J. Jekl[2]; R. Berkmortel[2]; [1]University of Western Ontario; [2]Meridian Technologies, Inc.

This paper summarizes the work performed, as part of a larger project, on a high-pressure die-cast AM60B magnesium alloy component. The ultimate goal of this project is to develop the capability to predict local mechanical properties from the die-casting parameters used during production. However, the variability of mechanical properties throughout a casting due to different local solidification conditions, as is the case in die-cast magnesium alloys, results in the inability to predict local mechanical properties from conventional methods. The work reported here reviews the relationships between local mechanical properties and local microstructural features developed for the die-cast AM60B component, that are applicable to any die-cast magnesium alloy. The results from this work indicate that the yield strength can be predicted from the average grain size through the casting thickness, and the local effective fracture strength from the size and relative location of the largest local area fraction of porosity.

11:30 AM
Grain Refinement of Mg-Al Alloys by Carbon Inoculation: *Yuanding Huang*[1]; Bin Liu[1]; Okechukwu Anopuo[1]; Norbert Hort[1]; Karl Kainer[1]; [1]GKSS Research Center

Grain refinement of magnesium alloys not only reduces the hot tearing and improves their mechanical properties, but also weakens the texture and improves their isotropic properties. In aluminium-free magnesium alloys, the element Zr is an effective nucleants to refine the microstructure and its mechanism of grain refinement is clear. In Al-containing magnesium alloys, the grain refinement by carbon inoculation was considered to be the best approach until now. However, the mechanism of grain refinement is still unclear. After inoculated by carbon or SiC particles, the grain size of as-cast Mg-Al alloys reduces largely. The grain refinement is mainly attributed to the enhanced nucleation of alpha-Mg on the surface of the ternary compound Al2MgC2. Experimental investigations also confirm that this ternary compound is unstable at room temperature and easily reacts with water to produce most likely the gas CH4 and the spinel phase MgAl2O4.

11:50 AM
A Systematic Study of the Grain Refinement of Magnesium by Zirconium: *Partha Saha*[1]; Katie Lolies[1]; Srinath Viswanathan[1]; Arun Gokhale[2]; Robert Batson[1]; [1]The University of Alabama; [2]Georgia Institute of Technology

Zirconium is well known as an excellent grain refiner for magnesium alloys that do not contain aluminum. While a number of studies on the grain refinement of magnesium alloys by zirconium have been reported in the literature, there is still some uncertainty about the exact mechanism of grain refinement. In this work, a Design of Experiments (DOE) approach was used for a systematic study of the grain refinement of magnesium by zirconium. Variables included the amount of zirconium, the pouring temperature, and the holding time prior to casting. Samples were poured into a special "hockey puck" mold designed to reproduce the conditions in permanent mold casting. Optical metallography and quantitative image analysis were used to measure the resultant grain sizes. The effect of the various factors on the measured grain size and the interaction among the various factors is discussed.

12:10 PM
Grain Refinement of AZ91 Alloy by Addition of Ceramic Particles: Dmitry Shepelev[1]; Julia Klemf[1]; Menachem Bamberger[1]; *Alexander Katsman*[1]; [1]Technion

The a-Al2O3 and SiC ceramic particles can serve as additives to refine the microstructure of Mg-based alloys. The Mg/a-Al2O3 and Mg/SiC pre-alloys were prepared using the new method developed in the present work. The ceramic particles were inserted into a molten Mg bath through a Mg-nitride layer formed at the surface of the liquid magnesium through which the nitrogen gas is blown. The particles of about 30-nm in size were placed in a porous alumina crucible and vacuum heat treated at 700°C. The liquid Mg penetrated through the porous walls of the crucible. The mixture was cooled to room temperature under a nitrogen atmosphere. The resulting Mg matrix contained about 15wt% evenly distributed particle agglomerates of about 0.5 µm. Alloy AZ91 was successfully grain refined using the pre-alloys developed. The grain size of the refined alloy, ~ 40µm, was about two times smaller than that of the base alloy.

Magnesium Technology 2010: Deformation Mechanisms

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Magnesium Committee
Program Organizers: Sean Agnew, University of Virginia; Eric Nyberg, Pacific Northwest National Laboratory; Wim Sillekens, TNO; Neale Neelameggham, US Magnesium LLC

Wednesday AM — Room: 612
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Sean Agnew, University of Virginia; Louis Hector Jr, GM R&D Center

8:30 AM
The Evolution of In-Grain Misorientation Axes (IGMA) during Deformation of Wrought Magnesium Alloy AZ31: *Young Chun*[1]; Chris Davies[1]; [1]Monash University

Understanding deformation mechanism is a prerequisite for the development of more formable magnesium alloys. We have developed a novel approach which is based on analysis of in-grain misorientation axes (IGMA) and allows identification of dominant slip system for a large number of grains. Based on this approach we investigated for rolled AZ31 the effects of orientations and temperatures on active deformation mechanisms, including slip, deformation twinning and kink banding. The IGMA analysis suggests that increasing rolling temperature promotes activation of prism < a > slip, which enhances the rollability of the plate favorably oriented for this slip mode. The approach also reveals orientation-dependent occurrence of kink banding and its crystallographic relationship with parent grain. It is concluded that IGMA analysis can be effectively used to study deformation mechanism in hcp metals, and also used as a criterion for substantiating the validity of some crystal plasticity models.

8:50 AM
Influence of Deformation Processing on the Tensile/Compressive Asymmetry in Wrought Mg-3Al-Zn Alloy: *Ran Liu*[1]; De Liang Yin[1]; Jing Tao Wang[1]; [1]Nanjing University of Science and Technology

Deformation anisotropy in a rolled Mg–3Al–1Zn alloy was investigated by mechanism-based modeling. Orientation factors for each slip and twinning systems in samples with typical rolled texture were conducted to find active deformation system, and the strain incrementals resulted from the activation of these deformation systems were accumulated for strain hardening and geometrical hardening evaluation. Modeling results indicate that the dominating deformation modes in samples with typical rolling texture are basal slip and [10-12] twinning, and the model results correspond quantitatively to the marked mechanical anisotropy of the rolled magnesium alloy.

9:10 AM
Importance of Crystallographic Texture of AZ31B Importance of Crystallographic Texture of AZ31B on Flow Stress Anisotropy and Tension-Compression Asymmetry: *Majid Al-Maharbi*[1]; David Floey[1]; Ibrahim Karaman[1]; Irene Beyerlein[2]; Ted Hartwig[1]; Laszlo Kecskes[3]; Suveen mathaudhu[3]; [1]Texas A&M University; [2]Los Alamos National Laboratory; [3]U.S. Army Research Laboratory

Crystallographic texture of AZ31B magnesium alloy processed using equal channel angular extrusion (ECAE) was found to play an important role in both flow stress anisotropy and tension-compression (T/C) asymmetry. In order to obtain different crystallographic textures, the alloy was ECAE processed following different conventional and hybrid ECAE routes. A viscoplastic self-consistent (VPSC) crystal plasticity model was employed to predict the texture evolution during ECAE. Despite the dynamic recrystallization taking place during the ECAE processing at 200°C and the continuous grain refinement with the number of ECAE passes, the crystallographic texture was successfully predicted up to four passes. The flow stress anisotropy and T/C asymmetry of the processed samples, were, then predicted using the same VPSC model coupled with a recently developed dislocation-based constitutive hardening law. The ramifications of these predictive capabilities on processing large AZ31B plates using ECAE for target crystallographic textures will be discussed.

9:30 AM
Mechanical Behavior of AZ31 Due to Texture and Microstructure: *David Foley*[1]; Majid Al-Maharbi[1]; K.T. Hartwig[1]; Ibrahim Karaman[1]; Laszlo Kecskes[2]; Suveen Mathaudhu[2]; [1]Texas A&M University; [2]US Army Research Lab

Achieving high strength in common Mg alloys requires phase, texture, and grain size distribution engineering. In order to understand the potential of SPD to control these parameters and to evaluate the mechanical behavior of the resulting materials, several studies were carried out. In AZ31, specimens were created with fixed texture and varied grain size, illustrating the grain size effect on yield, hardening, and mechanical anisotropy. Samples were also created with varied textures but fixed grain size distribution to evaluate these trends. In ZK60, varied thermomechanical processing has resulted in differing phase morphology and concentration. Finally, notable differences in texture development and microstructural refinement during deformation as well as general processability of these alloys will be discussed.

9:50 AM
Mechanical Anisotropy in Extruded Mg Alloy AM30: Brian Gerard[1]; Adam Niechajowicz[2]; Zbigniew Gronostajski[2]; *Wojciech Misiolek*[1]; [1]Lehigh University; [2]Wroclaw University of Technology

An industrial magnesium alloy AM30 extrudate was examined for microstructural gradients using metallographic techniques. Additionally, tensile samples were cut from the extrudate at different angles with respect to the extrusion direction. The tensile testing was performed at various high strain rates to study the influence of deformation anisotropy under automobile crash conditions. It was observed that the direction of tensile loading significantly impacted the yielding and fracture behavior as well as the dominant deformation mechanisms. These phenomena can be attributed to the highly anisotropic yielding behavior of magnesium hexagonal close packed crystals combined with a strong extrusion texture. Additionally, voids forming on specific twin planes were shown to significantly contribute to failure, which has been observed previously at low strain rates. The results of these experiments add to the knowledge base for determining the crashworthiness of structural magnesium alloy components.

10:10 AM
Implementation of the Anisotropy of Plastic Flow in Inverse Parameter Calculations of the Deformation Behavior of AZ31 Magnesium Alloy: Timo Ebeling[1]; *Christian Hartig*[1]; Rüdiger Bormann[1]; [1]Hamburg University of Technology

A better understanding of the texture evolution and anisotropic behavior is needed in order to improve the mechanical properties of magnesium wrought alloys. The approach is an investigation of the deformation mechanisms by model calculations. Therefore, room temperature tensile tests of AZ31 rolled sheets have been performed. The stress-strain behavior and the Lankford-coefficient have been measured.An inverse parameter calculation yielding information about deformation mode activities, texture evolution and mechanical properties was performed using a viscoplastic self-consistent model. Additional to the macroscopic hardening, the strain dependent Lankford coefficient, which reacts strongly on changes of the yield surface, was introduced into the modeling. The additional experimental input about the anisotropy of plastic flow yields a better insight into the mostly disregarded latent hardening of the deformation modes. It could be shown that the stress-strain behavior, the texture evolution and the Lankford-coefficient were simulated simultaneously under appropriate assumptions about the deformation modes.

10:30 AM
Tensile Mechanical Properties and the Ductile-To-Brittle Transition Behavior of the Mg-Li-Al-Zn Alloy: *Chung-Wei Yang*[1]; Truan-Sheng Lui[1]; Li-Hui Chen[1]; [1]National Cheng Kung University

The present study focuses on investigating the tensile mechanical properties and failure behaviours of the LAZ1021 Mg-Li alloy. The tensile tests of LAZ1021 specimens were performed at -25°C to 250°C, with a tensile strain rate of 1.67 × 10-3/s. The XRD analysis results represented that the microstructural characteristics of LAZ1021 was combined with the Mg-rich alpha-phase and the Li-rich beta-phase, and there was less phase composition change after tensile tests at various testing temperatures. The tensile strength and elongations were sensitive to the deformation temperatures. The total elongation was significantly increased from 4% at -25°C to about 55% above 100°C tensile testing temperatures. A significant ductile-to-brittle transition temperature (DBTT) was recognized at about 50°C. The failures, which occurred from brittle fracture with evident cleavage to ductile dimpled ruptures, is related to the transition of slip systems with increasing temperatures and the cavitation between alpha/beta-phase interface.

10:50 AM
The Influence of Sn and Pb Addition on the Tensile Properties of Mg Alloys: *Wei Gao*[1]; Hongmei Liu[1]; [1]The University of Auckland

A new Mg alloy system containing small amounts of Sn-Pb or Pb-Zr has been developed. These alloys possess exceptionally high ductility with good strength: the elongation reaches 20-28% at room temperature in as-cast state without any heat treatment. This type of cold deformation properties has not been reported with other Mg cast alloys. The small addition of Pb dramatically changed the microstructure of Mg-Sn alloys, forming small/round and well dispersed intermetallic phases. A special microstructure was also found in Mg-Sn-Pb alloy system: equiaxed grain boundaries and dendrite structures cross each other and independently exist in alloys. This microstructure cannot be explained by traditional solidification theories, but may have played an important role in improving ductility of these alloys. The development of this alloy system will open a door for Mg industry that cast alloy plate or sheet can be directly mechanically formed into net-shaped working parts.

11:10 AM
Room Temperature Tensile Anisotropy of Extruded Magnesium Plates: *Paul Krajewski*[1]; Adi Ben-Artzy[2]; Raj Mishra[1]; [1]General Motors; [2]Rotem Industries

The room temperature tensile behavior of four extruded magnesium plates: AZ31, AM50, ZM21, and AZ61 were evaluated at 0, 45, and 90 degrees to the extrusion direction. The low aluminum content alloys ZM21 and AZ31 exhibited significant anisotropy of ductility and flow strength. The 45 degree to the rolling direction showed the lowest yield strength and a ductility of over 25%. The higher aluminum content materials, AM50 and AZ61 exhibited no anisotropy of yield strength or ductility. EBSD was used to explain the differences in tensile behavior between the low Al and high Al content materials.

11:30 AM
Mechanical Properties and Microstructural Analysis of AXJ530 Magnesium Alloy Reinforced with Alumina Fibers: Bin Hu[1]; Liming Peng[1]; Bob Powell[2]; Anil Sachdev[2]; *Xiaoqin Zeng*[1]; [1]Shanghai Jiao Tong University; [2]General Motors Corporation

The creep-resistant magnesium alloy AXJ530 was reinforced with 15 volume percent, silica-bonded, Saffil fibers. The optimal squeeze casting parameters for infiltration of the fiber preforms were determined and the effects of reinforcement on the tensile and creep properties of the alloy were determined. Microstructural analysis of the composites, including the interface between the fibers and the AXJ530 matrix, was done. The results are discussed in terms of the shear lag theory for strengthening in composites.

11:50 AM
Very High Strain Rate Deformation of AZ31b Mg Alloys Using Split Hopkinson Pressure Bar: *Mehdi Sanjari*[1]; Amir Farzadfar[1]; Steve Yue[1]; Elhachmi Essadiqi[2]; [1]McGill; [2]CANMET-MTL

Nowadays, an understanding of strain rate dependence of material behavior is very important. The effects of strain rate on the deformation behavior of cubic materials have been studied extensively. However, high strain rate deformation of hexagonal materials has received relatively little attention. The present study considers the uniaxial compression behavior of as-cast AZ31B alloy at very high strain rates in the wide temperature range. A split Hopkinson pressure bar is used to attain strain rates in the range of 1000s-1. The results show that the microstructure is fully recrystallized at 250°C and strain rate of 103 s-1. The EBSD measurements show that most grains are oriented such that their c-axis is aligned with the compression direction. At higher strain rates such as 103 s-1, the basal poles split toward transverse directions indicating the activation of <c+a> slip systems because of increasing temperature due to more plastic and frictional work.

12:10 PM
Observation of Non-Basal Slip in Ductile Deformed MgY Alloys: Igor Schestakow[1]; *Stefanie Sandlöbes*[1]; Sangbong Yi[2]; Stefan Zaefferer[1]; [1]Max-Planck-Institut für Eisenforschung GmbH; [2]GKSS-Forschungszentrum - Magnesium Innovation Center (MagIC)

MgY clearly shows an enhanced room temperature ductility compared to pure Mg and other Mg alloys. The presented study of a Mg 3 wt-% Y alloy focuses on understanding the mechanisms for this ductility improvement by slip trace analysis, texture analysis based on electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM). Slip trace analysis on slightly RT-deformed MgY showed slip traces, which are consistent with second-order <c+a>-pyramidal slip. It has been reported that beside non-basal slip, {10-11} {10-12} double twinning might be responsible for the room temperature ductility enhancement. Texture and microstructure analysis of RT-deformed MgY showed, however, that besides double twinning, another texture-weakening deformation mode must be activated. Our TEM investigations showed a significant amount of non-basal dislocations in deformed MgY. The experimental results are discussed focusing on the mechanism effecting the observed activation of non-basal slip in MgY.

Materials in Clean Power Systems V: Clean Coal-, Hydrogen Based-Technologies, Fuel Cells, and Materials for Energy Storage: SOFC II

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS Structural Materials Division, TMS/ASM: Corrosion and Environmental Effects Committee, TMS: Energy Conversion and Storage Committee
Program Organizers: Xingbo Liu, West Virginia University; Zhenguo Yang, Pacific Northwest National Lab; K. Weil, Pacific Northwest National Lab; Mike Brady, Oak Ridge National Lab; Jay Whitacre, Carnegie Mellon University; Ayyakkannu Manivannan, National Energy Technology Laboratory; Zi-Kui Liu, Penn State University

Wednesday AM — Room: 211
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Zhenguo "Gary" Yang, Pacific Northwest National Laboratory; Jeffrey Fergus, Auburn University

8:30 AM Invited
Advanced Novel Interconnect Coatings for Hermetic Sealing and Mitigation of Cr Volatility in Planar SOFC Stacks: *Jung Pyung Choi*[1]; Scott Weil[1]; Matt Chou[1]; Jeff Stevenson[1]; Gary Yang[1]; Gordon Xia[1]; [1]Pacific Northwest National Laboratory

Low-cost, chromia-forming ferritic stainless steels have found widespread use in SOFCs, because of their low thermal expansion mismatch in high operating temperature. However, the volatile Cr-containing species, which originate from its oxide scale, can poison the cathode material in the cells and subsequently cause power degradation in the device. To prevent this, a conductive MnCo spinel coating has been developed. However this coating is not compatible with formation of hermetic seals between the interconnect frame component and the ceramic cell. Thus, a new aluminizing process has been developed to enable durable sealing, prevent Cr evaporation, and maintain electrical insulation between stack repeat units. This paper will present recent progress regarding these novel coatings and discuss some of the compatibility issues that arise when integrating both coatings into the same component.

9:10 AM Invited
Coating of Dense Oxide Layer on the Fe-Cr Alloys for Interconnects of Solid Oxide Fuel Cells: *Teruhisa Horita*[1]; Haruo Kishimoto[1]; Katsuhiko Yamaji[1]; Manuel Brito[1]; Harumi Yokokawa[1]; [1]AIST

Metallic interconnects are considered as interconnects of Solid Oxide Fuel Cells (SOFCs) operated at medium temperatures. The control of oxide scale growth is one of the critical issues for applying the Fe-Cr alloys. A coating of oxides is one candidates and several kinds of coatings have been examined by many authors. The present study adopted pulse laser deposition (PLD) method to deposit a dense (La,Sr)(Co,Fe)O3 (LSCF) on the Fe-Cr alloys. The oxide scale was formed between LSCF and Fe-Cr alloy. The microstructures, growth rates of oxide scale, and electrical conductivity of growth rate were discussed.

9:50 AM
Characterization of Mn-Co Electrodeposition for SOFC Interconnect Applications by QCM: *Junwei Wu*[1]; Ayyakkannu Manivannan[2]; Randall Gemmen[2]; Xingbo Liu[1]; [1]West Virginia University; [2]National Energy Technology Laboratory

(Mn,Co)3O4 spinel is one of the promising coating for solid oxide fuel cell (SOFC) interconnect application. Electroplating of alloys followed by oxidation offers a cost effective method to produce the desired spinel, and previous long term ASR and interconnect on-cell test which has been proved to be effective for interconnect application. The biggest barrier to Mn/Co co-deposition is the dramatic difference of deposition potentials of Mn (-1.18V) and Co (-0.28V), which makes it quite difficult to co-deposit two metals in thermodynamics aspect. In this work, fundamental aspects of Mn/Co co-deposition will be studied by quartz crystal microbalance (QCM). For comparison, pure Mn, Co depositions are studied as well. For all the depositions, mass gain follows the trend: Co > Mn-Co > Mn. Furthermore, SEM/EDX analysis shows Mn content increases with the applied voltage due to increased contribution to Mn deposition.

10:10 AM Break

10:20 AM Invited
Interactions between (Mn,Co)3O4 SOFC Interconnect Coating Materials and Chromia: *Jeffrey Fergus*[1]; Kangli Wang[1]; Yingjia Liu[1]; [1]Auburn University

Manganese cobalt oxides are promising coating materials for reducing chromium volatilization, and thus the associated cathode poisoning, from interconnect alloys in solid oxide fuel cells (SOFCs). Interaction between this coating and the oxide scale formed on the alloy during fuel cell operation can lead to changes in the coating composition and thus its performance. In this paper, the reaction between manganese cobalt spinel oxides and chromia is described. The reaction product consists of two layers. The layer in contact with chromia has two chromium ions per formula unit, i.e. (Mn,Co)Cr2O4, and grows by the diffusion of cobalt and manganese from (Mn,Co)3O4. In addition, chromium dissolves into (Mn,Co)3O4, which results in a second reaction layer. Both layers form the spinel structure, but there is a distinct difference between the growth mechanisms. When exposed to lower chromia activities, the (Mn,Co)Cr2O4 layer does not form even after long exposure times.

11:00 AM
Recent Progress in Cathode/Interconnect Contact Materials R&D for SOFCs at PNNL: *Gordon Xia*[1]; Zigui Lu[1]; Josh Templeton[1]; Gary Yang[1]; Jeffry Stevenson[1]; [1]Pacific Northwest National Laboratory

Contact materials for solid oxide fuel cell (SOFC) stacks are necessary for minimizing electrical contact resistances at the interfaces between interconnects and electrodes. In general, the contact materials should be electrically conductive, chemically and thermally stable, and capable to form robust bonds with adjacent SOFC components. At PNNL, we have been carrying out R&D on contact materials for a number of years. Our goal is to develop materials and methods for fabricating cost-effective and high performance contact layers between cathodes and interconnects during SOFC stacks assembling and operation. This paper will present the recent progress in our research and development on cathode/interconnect contact materials.

11:20 AM

The Evolution of Oxide Ridges during Scaling of Fe-22wt%Cr Alloys: *Jingxi Zhu*[1]; Laura Fernandez Diaz[2]; Gordon Holcomb[2]; Paul Jablonski[2]; Christopher Cowen[2]; David Laughlin[1]; Dave Alman[2]; Sridhar Seetharaman[2]; [1]Carnegie Mellon University; [2]National Energy Technology Laboratory

Oxide ridges were observed to form during the transient stage of the scale evolution in iron alloys containing 22 wt.% Cr at 800°C in dry air. The effect of La (120 and 290 ppm) and Ce (270 and 610 ppm) added during melt-stage processing were investigated. The surface oxidation process was imaged in-situ through a Confocal Scanning Laser Microscope (CSLM) and the results were correlated with post-experiment characterization through FEG-SEM and FIB-SEM combined with 3D reconstruction. It was found that the oxide ridges formed on top of the Cr-oxide scale and overlapped the intersections of the underlying alloy-grain boundaries with the Cr-oxide scale. Ridges were not observed on grain boundaries with misorientation angles less than 10º and consequently it is suggested that the boundaries of the top grains in the alloy serve as bottle necks for transport of Mn.

11:40 AM

The Possibility for IT SOFC Interconnector Material Used to Stainless Steel: Kee-Do Woo[1]; *MinSeok Moon*[1]; Eui-pyo Kwon[1]; Myeong-han Yoo[1]; Sang-hyuk Kim[1]; Duck-soo Kang[1]; [1]Chonbuk National University

IT SOFC(intermediate temperature solid oxide fuel cell) has low operating temperature than conventional SOFC system. In this study, the possibility of application of stainless steel as IT-SOFC materials was studied. An oxidation resistance layer on each differently surface treated specimen was investigated by using XRD, and FE-SEM. EDX result of STS430 showed that oxidation thickness of as polished, as received and sand blast samples were about 7.8µm, 12.8µm and 8.8µm, respectively. With increasing the exposed time from 100hr to 400hr, the oxide thickness of as polished, as received and sand blast samples increased to about 41.7µm, 17.7µm and 10.3µm, respectively. As a result, sand blast sample had very stabilized oxide film.

Modeling of Multi-Scale Phenomena for Batteries: Session I

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS/ASM: Computational Materials Science and Engineering Committee

Program Organizers: Adrian Sabau, Oak Ridge National Laboratory; Perla Balbuena, Texas A&M University, Artie McFerrin Department of Chemical Engineering; Venkat Subramanian, Tennessee Tech University, Department of Chemical Engineering

Wednesday AM — Room: 604
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Adrian Sabau, Oak Ridge National Laboratory; Venkat Subramanian, Washington University

8:30 AM Introductory Comments

8:35 AM

Predicting of Surface Morphology Defects in Electrochemical Storage Devices: *Adrian Sabau*[1]; Nancy Dudney[1]; [1]Oak Ridge National Laboratory

The demand for higher energy and power density batteries has created the need to understand the stability of interfaces and dynamic processes under realistic conditions.In the battery systems,there are regions with sharp composition gradients and reaction interfaces that are paramount to the understanding of the transport phenomena in electrode microstructures.Dendrite formation is a primary failure mechanism in lithium/polymer batteries.Most of the studies on dendrite initiation were based on experimental observations as a function of current,time,and surface features.Recently,it was found that solid electrolyte interphase(SEI)has an important role in dendrite initiation.Computer models could be one efficient tool to explore and understand the life-limiting phenomena in multi-component battery systems,which include SEI role on dendrite initiation. One of the main challenges is to develop new moving boundary models(MBM)for these nano-scale phenomena in order to bridge the multiple length-scale models for traditional MBM and novel interfacial models.

9:05 AM

Continuum and Multi-scale Modeling of Performance Curves and Capacity Fade in Lithium-Ion Batteries: Ravi Methekar[1]; Venkatsailanathan Ramadesign[1]; *Venkat Subramanian*[1]; Kejia Chen[2]; Richard Braatz[2]; [1]Tennessee Tech University, Department of Chemical Engineering; [2]University of Illinois at Urbana-Champaign

Mathematical models reported in the literature for capacity fade do not include all postulated mechanisms. Such a mathematical model, although highly desirable, has not been forthcoming due to (1) incomplete understanding of all of the capacity fade mechanisms, (2) lack of knowledge for the values of the model parameters in these mechanisms, (3) difficulties in obtaining these values due to cumulative non-separable effects of individual mechanisms occurring simultaneously, and (4) lack of efficient numerical solvers. A mathematical model reformulation for improving the computational efficiency of continuum models for lithium-ion batteries will be presented. The use of these efficient algorithms to model capacity fade and to identify optimal operational strategies and materials design will be presented. In addition, the development and implementation of a Kinetic Monte Carlo (KMC) and coupled KMC-continuum multi-scale model to quantify the effect of surface-reaction mechanisms and heterogeneity at the solid-electrolyte interface will be presented.

9:35 AM

Diffusion and Phase Transformations in Lithium Ion Battery Anodes from First Principles: *Jishnu Bhattacharya*[1]; Anton Van der Ven[1]; [1]University of Michigan

Lithium ion battery electrodes consist of intercalation compounds that accommodate Li ions in interstitial sites. Charge-discharge rates and reversibility depend sensitively on diffusion and the kinetics of first-order phase transformations. Here, we study Li diffusion and phase transformation mechanisms in titanates, a class of transition metal oxides that are increasingly considered as promising candidate anodes for high rate batteries. Li-diffusion occurs primarily in the non-dilute regime. Therefore, interactions among Li ions are important in determining diffusion mechanisms and rates. To predict the composition dependence of the Li diffusion coefficients from first-principles, we evaluate Kubo-Green expressions using the cluster expansion technique in kinetic Monte Carlo simulations. We find that diffusion coefficients depend sensitively on Li composition and titanate crystal structure. These calculated diffusion coefficients can then be used in continuum simulations of electrode dynamics. Migration of interfaces during first-order phase transformations will also be discussed.

10:05 AM Invited

The Solid-Electrolyte-Interface Processes in Lithium-Ion Battery by Atomistic Simulations: *Ken Tasaki*[1]; [1]Mitsubishi Chemical USA

The solid-electrolyte-interface (SEI) processes in lithium-ion battery cells critically affect the battery performance such as the cycle life, the cell life, and the safety; yet, little is understood on the SEI film characteristics, the film formation mechanism and others. In this report, we focus on the SEI processes on the anode electrode side, trying to shed light into their complex nature through atomistic simulations. The SEI film is a heterogeneous system consisting of organic as well as inorganic salts in both amorphous and crystalline phases. This makes atomistic simulations challenging. We show experimental observations for a wide range of salts can be reproduced, at least qualitatively, through relatively simple manipulation of force field parameters based on DFT calculations. The subjects we discuss in our report will include the solubility of SEI film components in organic solvent and the thermodynamics on the Li insertion to graphite.

10:50 AM Concluding Comments

Modeling, Simulation, and Theory of Nanomechanical Materials Behavior: Physics of Defects, Dislocation Nucleation and Fracture I

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS/ASM: Computational Materials Science and Engineering Committee, TMS: Nanomechanical Materials Behavior Committee
Program Organizers: Thomas Buchheit, Sandia National Laboratories; Sergey Medyanik, Washington State Univ.; Douglas Spearot, University of Arkansas; Lawerence Friedman, Penn State University; Edmund Webb, Sandia National Laboratories

Wednesday AM   Room: 304
February 17, 2010   Location: Washington State Convention Center

Session Chairs: Sulin Zhang, The Pennsylvania State University; Sergey Medyanik, Washington State University

8:30 AM Invited
Nanoscale Modeling of Fracture: *W. Curtin*[1]; S. Chakravarthy[1]; [1]Brown University

We apply the plane-strain-dislocation-dynamics (DD)/cohesive-zone (CZ) model to investigate the fracture of high-strength metal alloys bonded to elastic substrates, with application to thermal barrier coatings. In these systems the plastic zone size is on the order of 50nm and the atomistic cohesive zone lengths are sub-nanometer, so that the discreteness of the dislocations may be essential to capturing the toughening mechanisms. We use a new set of methodological tools that overcome computational and conceptual issues associated with prior DD implementations. We then predict the toughness as a function of the internal metal structure (obstacle strengths and spacings) at a fixed macroscopic yield stress, and as a function of the nanoscale cohesive zone parameters. The role of crack-tip dislocation nucleation is also explored. Comparisons of our results to predictions from strain-gradient plasticity are made, with the goal of identifying material features that establish the gradient length scale in this problem.

9:00 AM
Understanding Scaling Relations in Fracture and Mechanical Deformation of Single Crystal and Polycrystalline Silicon by Performing Atomistic Simulations at Mesoscale: Hansung Kim[1]; *Vikas Tomar*[1]; [1]University of Notre Dame

In past, several methods have been developed to overcome the limitation of time scale in atomistic simulations such as molecular dynamics (MD) time acceleration methods, Voter et al. 2002, and Hybrid Monte Carlo method (HMC), Mehlig et al. 1992 and Tomar 2007. However, till now it has not been possible to atomistically investigate meso and micro-scale phenomenon using MD simulations at continuum time scale. In this talk, a new atomistic method is developed to increase time step and size of MD simulations and used to investigate mechanical deformation and dynamic fracture in single crystal and polycrystalline silicon. In this method, dynamic equivalent crystal lattices are generated to represent a classical analogue of the statistical mechanical description of the underlying material. By using the method, we found that the length scale can increase up to 200 times and time scale up to 500 times.

9:20 AM
Effects of Geometry, Mode Mixity, and Temperature on Dislocation Nucleation in Strained Electronics: Tianlei Li[1]; Jinhaeng Lee[1]; *Yanfei Gao*[1]; [1]University of Tennessee

Dislocation loops may be nucleated from sharp geometric features in strained micro- and nano-electronic devices. This process is investigated by a dissipative cohesive interface model which treats the dislocation core as a continuous, inhomogeneous lattice slip field. As a representative example, we calculate the critical stress for dislocation nucleation from the edges/corners of a rectangular Si_3N_4 pad on a Si substrate as a function of geometric parameters such as the length-to-height ratio and the three-dimensional shape of the pad. The shapes of the dislocations are also simulated. An important observation arises from the mode mixity of the singular stress fields near the edge. The relationship between the critical stress intensity factor and the mode mixity can be determined from this explicit model of dislocation nucleation process zone. The dependence of both critical load and activation energy on modulus mismatch as characterized by Dundurs parameters will be presented.

9:40 AM
Analysis of Genealized Stacking Fault Energy for FCC Fe-Mn Alloys Using Molecular Dynamics Simulation: *Minho Jo*[1]; Y. M. Koo[1]; S. K. Kwon[1]; [1]Graduate Institute of Ferrous Technology, Pohang University of Science and Technology

Atomistic calculations for the <112>-generalized stacking fault (GSF) energy curve are performed for various fcc Fe-Mn alloys making use of molecular-dynamics simulations. A modified embedded atom method potential is used to model atomic interactions. The <112>-GSF energy curves are analyzed into stacking fault energy (SFE), unstable stacking fault energy (USFE), twinning fault energy (TFE), and unstable twinning fault energy (UTFE). With the energy terms, we tried to explain various deformation behavior of Fe-Mn system. It is suggested that the difference of USFE and UTFE barriers determines the next procedure after occurring one stacking fault, e.g., twin broadening or additional stacking fault. If USFE is lower than UTFE, additional stacking fault will be induced at different plane regardless of SFE. Otherwise, twin boundary propagates enlarging twin region.

10:00 AM Break

10:20 AM Invited
Size Effect on the Fracture Behaviors of Si Nanowires in Tension: *Wei Cai*[1]; Keonwook Kang[1]; [1]Stanford University

We performed Molecular Dynamics (MD) simulations of [1 1 0]-oriented Si nanowires (NWs) described by the modified embedded-atom-method (MEAM) potential under uniaxial tensile loading at a constant strain rate until failure. We found that the brittle or ductile fracture behavior of the NWs depends not only on the temperature but also on the NW diameter. Thick NWs break by crack nucleation and growth on the (110) plane at low temperature (a “brittle” mechanism) and by dislocation-mediated slip on {111} planes at high temperature (a “ductile” mechanism). Surprisingly, NWs with diameter less than 4 nm break by the “brittle” mechanism regardless of the temperature. The observed size and temperature dependence of fracture behavior is explained in terms of the competition between crack and dislocation nucleation from the NW surface.

10:50 AM
Lattice Misorientation Patterns and Strain Gradient Effects in Single Crystals under Spherical Indentation: *Yanfei Gao*[1]; B. Larson[2]; G. Pharr[1]; [1]University of Tennessee; [2]Oak Ridge National Laboratory

The ability to quantitatively predict dislocation microstructure and its evolution on mesoscopic length scales is a critical step towards developing a mechanistic understanding of small scale crystal plasticity. The three-dimensional measurements of lattice rotation and elastic strain fields with sub-micron resolution by a x-ray structural microscopy can be used to compute the lattice curvature and the dislocation density tensor. The modeling effort adopts a strain-gradient crystal plasticity theory in which the extra hardening to the slip strength arises from the geometrically necessary dislocations. Experimental/modeling comparisons suggest that when the ratio a/R (with contact radius a and indenter radius R) is less than about 0.2, the lattice rotation pattern is determined primarily by the crystallographic orientations, slip systems, and indenter shape, but is insensitive to the gradient effects. The magnitude of lattice misorientation angle can be estimated from the ratio a/R for spherical indenters or the pyramidal indenter angle.

11:10 AM Invited
Nanoscale Fracture in Graphene: *Sulin Zhang*[1]; [1]The Pennsylvania State University

The nanoscale fracture of a monolayer graphene is governed by the competition between bond breaking and bond rotation at a crack tip. We were able to precisely control the cracking pathways in atomistic simulations of graphene fracture. This was achieved by utilizing the lattice trapping effect which arises intrinsically due to the discrete nature of crystal lattice. We identified a novel fracture mechanism, involving the fracture paths of alternating bond rotation and rupture. The results demonstrate that mechanical cracking can create strain-engineered fracture edges with atomic-scale morphologies, providing a structural basis of tailoring the electronic properties of graphene either intrinsically or by further functionalizing the edges.

Neutron and X-Ray Studies of Advanced Materials III: Strain and Dislocation Gradients from Microdiffraction II

Sponsored by: The Minerals, Metals and Materials Society, ASM International, TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee, TMS: Titanium Committee
Program Organizers: Rozaliya Barabash, Oak Ridge National Laboratory; Jaimie Tiley, Air Force Research Laboratory; Erica Lilleodden, GKSS Research Center; Peter Liaw, University of Tennessee; Yandong Wang, Northeastern University

Wednesday AM Room: 303
February 17, 2010 Location: Washington State Convention Center

Session Chairs: Dean Haeffner, Argonne National Laboratory; Klaus-Dieter Liss, Australian Nuclear Science and Technology Organisation

8:30 AM Keynote
Strain and Dislocation Density in Barium Titanate by Synchrotron and Laboratory X-Ray Diffraction: *Davor Balzar*[1]; [1]University of Denver

Ferroelectrics are attracting much attention because of their growing use by electronics industry. Diffraction provides means of determining both strains (stresses) and defects. We studied microstructural changes upon poling of polycrystalline BaTiO3 using high-resolution synchrotron x-ray diffraction. We report evidence for a significant increase of defects density with an associated strain-energy increase. This implies that the application of an external poling field generates defects in the structure and increases the internal stress. Possible consequences in both bulk and thin-film applications include accelerated aging and microcracking.

9:00 AM Invited
Using X-Ray Microbeams to Measure Complete Strain Tensors from Dislocation Cell Structures in Deformed Cu: *Michael Kassner*[1]; Peter Geantil[1]; Lyle Levine[2]; Bennett Larson[3]; Jon Tischler[3]; [1]University of Southern California; [2]National Institute of Standards and Technology; [3]Oak Ridge National Laboratory

Previous studies by our group produced the first quantitative, spatially resolved measurements of elastic strains from individual dislocation cell walls and cell interiors in heavily deformed metals. The measurements demonstrated that these dislocation structures were under significant, widely varying internal stresses of opposite sign. However, these investigations only measured elastic strains in the axial (deformation) direction. We have now initiated measurements of diffraction line profiles for multiple independent reflections from spatially resolved, submicrometer sample volumes, which make it possible to extract all six elements of the strain tensors from spatially resolved dislocation cell interiors. The experimental and data analysis techniques for these measurements will be described, along with preliminary results. These measurements will provide critical data for validating and guiding the development of detailed dislocation-based simulations and models for dislocation structure evolution.

9:20 AM
Microstructure, Mechanical Behavior and Deformation Mechanisms of Nanocrystalline Ni-50wt%Fe: *Steven Van Petegem*[1]; Julien Zimmermann[1]; Stefan Brandstetter[2]; Xavier Sauvage[3]; Marc Legros[2]; Bernd Schmitt[1]; Helena Van Swygenhoven[1]; [1]Paul Scherrer Institut; [2]CEMES-CNRS; [3]University of Rouen

In order to understand the elastic and plastic deformation properties of nanocrystalline metals we have developed an in situ synchrotron x-ray-diffraction technique which allows the simultaneous measurement of many diffraction peaks continuously during mechanical testing, providing a direct link between the evolving microstructure and the macroscopic mechanical data. Here we present recent results obtained for electrodeposited Ni-Fe with a nominal iron content of 50%. The microstructure of this alloy is characterized by a narrow grain size distribution with a mean value of 10nm. Uni-axial mechanical tensile tests indicate that Ni-Fe exhibits a transient regime during reloading or after transient testing. This regime is characterized by an upper or lower yield point. Such a yield point is not observed during continuous loading. Furthermore the strain rate sensitivity is relatively low. In-situ x-ray diffraction experiments reveal a strong relaxation effect during initial loading in the microplastic regime.

9:35 AM Invited
X-Ray Diffraction Microscopy Studies of Microstructure Responses: Christopher Hefferan[1]; Shui Fai Li[1]; Ulrich Lienert[2]; Anthony Rollett[1]; Greg Rohrer[1]; *Robert Suter*[1]; [1]Carnegie Mellon University; [2]Argonne National Laboratory

We present progress and future trends in synchrotron high energy x-ray diffraction microscopy studies of microstructure evolution. Differential thermal annealing in high purity aluminum has been observed and compared to predictions of curvature driven grain growth, both on the coarse grained level of the MacPherson-Srolovitz equation and on the level of individual boundary motions. Future work will include the combination of microstructure mapping with 1) tomography to detect and correlate void formation with microstructural features upon strain application and 2) strain tensor measurements to generate maps of ensembles of grains including geometry, neighborhood, and stress states. These measurements will allow validation of polycrystal plasticity models of materials response. Large volumetric data sets can be used as starting states in computations and computed responses compared to experimental observations. The capabilities described are applicable to a wide variety of materials; derived understanding should lead to improved materials design and prediction of properties.

9:55 AM
Thermo-Mechanical Processing in a Synchrotron Beam: *Klaus-Dieter Liss*[1]; [1]Australian Nuclear Science and Technology Organisation

Well collimated, high energy X-rays of 90 keV from synchrotron sources have been used to study metals undergoing plastic deformation in-situ, in real time and in the bulk of the materials. The spottiness of poorly illuminated Debye-Scherrer rings showing reflections from individual crystallites is analyzed to obtain grain statistics, mosaic spread and orientation. Upon cold deformation, coarse grained materials show fingerprints of sub-grain formation, grain rotation, grain refinement and the evolution from a single grain into the asymptotic texture. Heating of metals under continuous load drives the observation through the regimes of phase transformation and grain relationships therein, grain coarsening, dynamic recovery and dynamic recrystallization. The paper points out these different phenomena which were observed without precedence.

10:10 AM Invited
Correlation of X-Ray Diffraction Examination of Recovery in Cold-Rolled Aluminum with Dynamic Dislocation-Defect Analysis: *Shig Saimoto*[1]; Joyce Cooley[1]; [1]Queen's University

X-ray line-profile analysis tends to become one of model-in and model-out, even for pure metals. One way to delineate contributing effects is to correlate the changes with other complimentary methods during recovery. The role of point defects and their recovery has resulted in a suggestion that examination of the diffuse background scattering can reveal their presence. This methodology was pursued at recovery temperatures below 200 °C where point defects, small loops and stacking fault tetrahedra's are reported to anneal out. Furthermore the applicability of using the typical 2-theta diffraction scanning with K-alpha one and two to qualitatively reveal the recovery process was examined in comparison with the use of a four-bounce monochromator. The results indicate that recovery of the background scattering is related to the presence of geometrically necessary boundaries rather than point defects or loops. This observation suggests copious presence of stacking faults within these boundaries.

10:30 AM Break

10:40 AM Invited
FSP-Induced Plastic Deformation and Elastic Strains in Individual Dendrites of the Ni-Based Superalloy from X-Ray Microdiffraction: *Oleg Barabash*[1]; Rozaliya Barabash[1]; Gene Ice[1]; Zhili Feng[1]; [1]Oak Ridge National Laboratory

Spatially-resolved X-ray micro-Laue diffraction and SEM were used to study FSP-induced local structural transformations in the individual dendrites of the Ni -based superalloy near the boundary between the TMAZ and the SZ. Material behavior is distinct in the TMAZ and the SZ. Plastic deformation of individual dendrites with the formation of shear bands takes place in the TMAZ. Bending of the dendrites in the {111} plane and rotation towards <011> pole is observed. Due to dislocations movement and interactions at the FSP-induced high temperatures, they rearrange with the formation of small-angle boundaries. Elastic strain and GNDs density tensors within the individual dendrites are determined from the analysis of micro-Laue diffraction. Severe plastic deformation and recrystallyzation takes place in the SZ. Dendrite structure is completely destroyed in the SZ in contrast to the TMAZ The formation of the so called "onion rings" structure with the bimodal grain size distribution is found.

11:00 AM Invited

Synchrotron Microdiffraction Analysis of the Microstructure of Cryogenically Treated High Performance Tool Steels Prior to and after Tempering: *Ning Xu*[1]; Andrea Gerson[1]; Giuseppe Cavallaro[1]; [1]ACeSSS (Applied Centre for Structural and Synchrotron Studies)

The phase transformation and strain changes within cryogenically (-196°C) treated high performance tool steels (AISI H13) before and after tempering have been examined using both laboratory XRD and synchrotron microdiffraction. The martensitic unit cell was found to have very low tetragonality as expected for low carbon steel. Tempering resulted in the diffusion of excess carbon out of the martensite phase and consequent unit cell shrinkage. On tempering the martensite became more homogeneous for cryogenically treated samples as compared to those had not been tempered. The effect was most pronounced for the rapidly cooled sample which was the least homogenous sample prior to tempering but was the most homogenous sample after tempering. This suggests that considerable degree of disorder due to rapid cryogenic cooling results in the beneficial release of micro-stresses on tempering thus possibly resulting in the improved wear resistance and durability observed for cryogenically treated tool steels.

11:20 AM Invited

Materials Studies Using High-Resolution Laue X-Ray Microdiffraction: *John Budai*[1]; Wenjun Liu[2]; Jon Tischler[1]; [1]Oak Ridge National Laboratory; [2]Argonne National Lab

Synchrotron microdiffraction facilities such as the scanning, polychromatic microscope at the Advanced Photon Source (beamline 34ID-E) provide unique opportunities for structural studies of a wide range of advanced materials. At this focused microbeam facility, depth-resolved Laue diffraction patterns are analyzed with automated software, to produce 3-D maps of the local crystal structure, lattice orientation and strain tensor. This talk will illustrate how new spatially-resolved information can be obtained from materials systems ranging from 1-D nanostructures to bulk 3-D polycrystals. For example, studies of luminescent 1-D nanowires have revealed new crystal structures and provided local information such as the preferred growth axes. In 3-D materials, structural investigations have included nondestructive studies of thermal grain growth in polycrystalline aluminum, lattice parameter changes in ferroelectrics and local phase separation in complex manganite crystals. Support at ORNL, UT-Battelle by DOE-BES, Materials Sciences and Engineering Division; UNI-XOR support at APS by DOE-BES.

11:40 AM

Wear Properties of Single Phase Ti Alloys and Surface Damage Characterization by X-Ray Diffraction: *Eri Miura-Fujiwara*[1]; Hisashi Sato[1]; Gene Ice[2]; Yoshimi Watanabe[1]; [1]Nagoya Institute of Technology; [2]Oak Ridge National Laboratory

Characteristic deformation behavior due to wear in single phase Ti alloys was investigated using a glancing angle powder diffraction method with X-ray microbeam. Wear test was performed by a ball-on-disc test in artificial saliva at 310 K. From the results of our previous study, alpha phase (hcp) peaks and beta phase (bcc) peaks changed in different ways when wear damage was introduced in Ti-6Al-7Nb, alpha + beta Ti alloy for biomedical applications. That is, alpha peaks showed peak broadening and orientation alignment, and beta peaks showed peak broadening and peak shift. Thus, the results infer that diffraction peaks of single phase could behave likewise. In this study, we investigated single alpha or beta phase Ti alloys. Similar peak broadening or peak shifts as alpha + beta Ti alloy were confirmed in commercial purity Ti and Ti-Al-Zr-Mo-Nb alloy after wear test.

11:55 AM Invited

Polychromatic X-Ray Microdiffraction (PXM) Studies of Stress Corrosion Cracking (SCC) in Alloy 600: *Marina Suominen Fuller*[1]; Jing Chao[1]; N. Stewart McIntyre[1]; Sridhar Ramamurthy[1]; Leo Lau[1]; Roger Newman[2]; Anatolie Carcea[2]; Renfei Feng[3]; [1]University of Western Ontario; [2]University of Toronto; [3]Canadian Light Source Inc.

Stress corrosion cracking (SCC) is known as an active degradation mechanism in steam generators used in both CANDU and PWR nuclear reactors. Alloy 600 has been used as the primary steam generator (SG) tubing material and is prone to SCC. To predict the onset of cracking under the SG operating conditions requires that the interplay of mechanical and chemical behaviours of these materials be thoroughly understood. The synchrotron-based Polychromatic X-ray Microdiffraction (PXM) method will be used to follow the strain distributions around cracks in stressed Alloy 600 C-rings exposed to (a) water vapour/hydrogen and (b) caustic environments. Some of the first PXM results from the new VESPERS beamline at the Canadian Light Source in Saskatoon, SK, Canada, will be shown.

12:15 PM

Crystal Distortion Gradient in the Vicinity of a Grain-Boundary in Plastically Deformed Bicrystals: *Gael Daveau*[1]; Benoit Devincre[1]; Thierry Hoc[2]; Odile Robach[3]; [1]LEM-CNRS/ONERA; [2]MSSMat-Centrale Paris; [3]NRS/CEA-Grenoble

A dislocation density based model [1] developed for fcc single crystal is extended for the simulation of strain hardening of polycrystal materials. Crystal rotation and elastic strain in a strained copper bicrystal were measured by X-ray microdiffraction. Existence of a strain gradient in the vicinity of the grain boundary at low plastic deformation is shown. Dislocation dynamics simulations are used to investigate the influence of dislocation density gradient on the diffraction pattern. From those calculations, a decrease of the dislocation mean free path is defined as a function of the boundary distances. A modified crystal plasticity constitutive law accounting for the influence of grain boundary is proposed. Finally, a comparison between the results of finite elements simulations and experiments is made.[1] Devincre, Hoc, Kubin, Science, 320 (2008) p 1745-1748.

12:25 PM

Grain Rotation and Texture Evolution in Cubic Polycrystals Determined by Synchrotron X-Ray Diffraction: *Kun Yan*[1]; Klaus-Dieter Liss[1]; Rian Dippenaar[2]; [1]The Bragg Institute; [2]University of Wollongong

By high energy synchrotron X ray diffraction, the evolution of microstructures during the compression of copper with different grain sizes were traced respectively. The grain refinement and mosaic spread of sub-grain were observed dynamically from the movie of 2D diffraction patterns as well as the diffraction profile broadening, the anisotropic grain orientations were obtained with numerical analysis. Complementary neutron diffraction was employed for the ex-situ texture measurement, which approve the effects of grain rotation on the formation of texture. Relation between lattice strain and grain refinement rate was analyzed with various loading condition. The results fulfill the understanding of the evolution of grain orientation and slip mechanism during compressive deformation.

12:35 PM

2010 JIM International Scholar Award Winner: **Development of Coherent X-Ray Diffraction Microscopy and Its Application in Materials Science**: *Yukio Takahashi*[1]; Y. Nishino[2]; T. Ishikawa[2]; K. Yamauchi[1]; E. Matsubara[3]; [1]Osaka University; [2]RIKEN SPring-8 Center; [3]Kyoto University

Coherent X-ray diffraction microscopy (CXDM) is a novel technique for reconstructing the electron density distribution of a sample, which has attracted much attention as a new tool for analyzing the nanostructures of metallic materials. CXDM has great potential as a technique for structural studies of metallic materials because it is a nondestructive method and is applicable to samples of micrometer thickness. Until now, we have applied CXDM to the mesoscopic structure analysis of a precipitation-hardened aluminum alloy and to the in-situ observation of electromigration voids in a Cu thin line. Recently, aiming towards the development of higher-resolution CXDM, we have developed a high-resolution CXDM using synchrotron X-rays focused by total reflection mirrors, and have achieved 3 nm resolution. We have successfully reconstructed the three-dimensional electron density distribution of a shape-controlled gold nanoparticle using the high-resolution diffraction microscope.

The present method is the key technology for realizing single-pulse diffractive imaging using X-ray free electron lasers.

Nuclear Energy: Processes and Policies: Material Behavior

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS/ASM: Nuclear Materials Committee, TMS: Public and Governmental Affairs Committee
Program Organizers: Brajendra Mishra, Colorado School of Mines; Aladar Csontos, U.S. Nuclear Regulatory Commission; Stuart Maloy, Los Alamos National Laboratory; Jeremy Busby, Oak Ridge National Laboratory; Sue Lesica, U.S. Department of Energy's Office of Nuclear Energy

Wednesday AM Room: 201
February 17, 2010 Location: Washington State Convention Center

Session Chairs: Stuart Maloy, Los Alamos National Laboratory; Jeremy Busby, Oak Ridge National Laboratory

8:30 AM Keynote
Future of Nuclear Energy Research and Development: *Sue Lesica*[1]; [1]U.S. Department of Energy's Office of Nuclear Energy
Abstract not available.

9:05 AM
A Study of the Initial Effects of Irradiation on Nanocluster Stability on ODS Steel: *Alicia Certain*[1]; Jim Bentley[2]; Michael Miller[2]; Jeremy Busby[2]; Robert Ulfig[3]; Todd Allen[1]; Kevin Field[1]; [1]University of Wisconsin-Madison; [2]Oak Ridge National Laboratory; [3]Imago Scientific Instruments
Oxide dispersion strengthened ferritic/martensitic steels, otherwise referred to as nano-featured alloys (NFAs), are considered for fission and fusion applications for their improved high-temperature properties and the assumed radiation resistance. This paper reports on work aimed at understanding the irradiation performance of NFAs and attempts to determine the current boundaries in studying the very small and complex nanoclusters of this material with advanced imaging and compositional techniques, and to apply these techniques to observe the initial evolution in composition and/or microstructure of the nanoclusters. NFAs were irradiated to low dose with protons in the temperature range of 400-700°C and doses ranging from 1 to 10 dpa. Samples were investigated by energy-filtered TEM, STEM/EDS, and atom probe tomography. The size range (~0.5 nm to 30 nm diameter) and the relative inhomogeniety of the nanocluster distribution make using complimentary analysis techniques essential to a complete understanding of the nanocluster evolution under irradiation.

9:30 AM
Fracture and Impact Properties of HT-9 Steel Irradiated to High Dose in FFTF: *Thak Sang Byun*[1]; Stuart Maloy[2]; [1]Oak Ridge National Laboratory; [2]Los Alamos National Laboratory
Fracture and impact properties were investigated for the ACO-3 duct (made of HT-9) irradiated in the Fast Flux Test Facility (FFTF). Small Charpy impact specimens with the dimensions of 3×4×27mm and disk compact tension (DCT) fracture specimens with 12.7mm diameter and 3mm thickness were machined from various positions of the ACO-3 duct that had been irradiated in FFTF up to a total dose of 155 dpa and irradiation temperatures were in the range of 370–510ºC. The impact tests were performed in a 25J capacity tester in the temperature range from -50 to 350ºC, and the fracture toughness tests performed at room temperature, 250, and the irradiation temperature in a servo-hydraulic testing machine. The ductile-to-brittle transition temperature (DBTT) increased with dose, while the upper shelf energy decreased with dose and reached levels lower than 5J. These data will be summarized and compared to previous fast reactor test data.

9:55 AM
In-Plane Anisotropy in Microstructure and Mechanical Behavior of Alloy 617 Following High Temperature Aging: *Kun Mo*[1]; Gianfranco Lovicu[2]; Hsiao-ming Tung[1]; Xiang Chen[1]; James Stubbins[1]; [1]University of Illinois; [2]University of Pisa
Alloy 617 is considered as a leading material used for next generation nuclear power plant, due to its good corrosion resistance and exceptional high-temperature strength. In the present work, the effects of long-term aging (up to 3000 h) at 900°C and 1000°C on the microstructure and associated mechanical properties were investigated. Specimens from the rolling plane and transverse plane were selected to study the anisotropic effect, which was originally induced by intermetallic inclusions from the hot rolling processing. Microstructure characterization by transmission electron microscope (TEM) and scanning electron microscope (SEM) revealed the precipitation evolution processes for different aging conditions. Precipitate type, size, location and coherency were investigated. Hardness and tensile tests showed that the influence of the in-plane anisotropy was significant during the aging process, which may be attributed to diffusion-controlled coarsening of the precipitates.

10:20 AM Break

10:35 AM
MaRIE; A Proposed Materials Facility at Los Alamos National Laboratory: *Mark Bourke*[1]; [1]Los Alamos National Laboratory
Los Alamos National Laboratory is currently engaged in the definition of a facility called MaRIE (Matter-Radiation Interactions in Extremes). It is being conceived as a world class national user facility that will provide unique measurements of material performance under extreme radiation conditions and during dynamic shock events on, among others, materials of relevance to the fission and national security communities respectively. Current objectives include; in situ measurement of materials response in a fast reactor level neutron fluence (with complementary ex situ PIE capabilities), in situ measurements of strain with microstructural spatial resolution and nanosecond temporal resolution during explosive shock events and provision of state of the art synthesis and characterization tools. The concept anticipates the increasing role that control science is expected to play in materials research when compared to observation science. Experimental capabilities are being considered that will most usefully inform models enabled by recent advances in computational capability.

11:00 AM
Microstructural Evolution in Friction Stir Welded MA956 and 14YWT: *Michael West*[1]; Bharat K. Jasthi[1]; William J. Arbegast[1]; David T. Hoelzer[1]; [1]South Dakota School of Mines and Technology
Friction stir welding presents a unique opportunity for joining oxide dispersion strengthened (ODS) alloys. This research presents results of friction stir welding the high temperature ODS alloys MA956 and the nanostructured ferritic alloy 14YWT. Studies focus on alternative thermal strategies such as induction preheating as a way of lowering process forces. The effect of process parameters on resulting particle dispersion and microstructure are discussed.

11:25 AM
The Behavior of Precipitate Strengthened Steels under Irradiation: *Peter Hosemann*[1]; Erich Stergar[2]; Stuart Maloy[1]; Harald Leitner[2]; Andrew Nelson[1]; [1]LANL; [2]University of Leoben
Oxide dispersion strengthened alloys are known to be radiation tolerant and usable up to high temperature and dose. The key to creating materials with extraordinary radiation tolerance is to allow the created defects to annihilate on defect sinks such as nano precipitates. Here new heats of the alloy 14YWT were made and irradiated using a low energy proton beam. The post irradiation examination results are presented on those materials.Maraging steels are known to form intermetallic precipitates at a proper heat treatment. Here we exposed a Co free maraging steel (Corrax) (aged and not aged) to ion beam irradiation and performed PIE to investigate the effectiveness to reduce radiation damage in the material by these intermetallic particles. Post irradiation nanoindentation showed a hardness increase of the maraging steel to the same level as a 500C heat treatment would achieve.

11:50 AM
In Situ Synchrotron Study and Computer Modeling of Advanced Nuclear Structural Alloys: *Meimei Li*[1]; Jonathan Almer[1]; Ken Natesan[1]; David Rink[1]; [1]ANL
Advanced materials are often multi-component alloy systems with many different phases. The development of such complex alloy systems has historically been a long process from initial trials to implementation due to lack of a fundamental understanding of the physical mechanisms controlling mechanical responses. This development process can be significantly shortened with advanced computer simulations tools coupled with advanced experimental techniques. In this paper, we will present recent findings on the applications of

in situ synchrotron x-ray diffraction to the study of the temporal evolution of structure and phases during high temperature thermo-mechanical processing in advanced ferritic-martensitic steels. Computer modeling by Thermo-Calc was used to calculate phase equilibria and diffusion-controlled precipitation and coarsening kinetics. Experimental data of phase analysis are compared with modeling results to understand the microstructure development under thermo-mechanical conditions and its impact on the development of high-performance structural alloys for advanced nuclear energy applications.

Pb-Free Solders and Emerging Interconnect and Packaging Technologies: Alloy Development

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Electronic Packaging and Interconnection Materials Committee
Program Organizers: Kwang-Lung Lin, National Cheng Kung University; Sung Kang, IBM; Jenq-Gong Duh, National Tsing-Hua University; Laura Turbini, Research In Motion; Iver Anderson, Iowa State University; Fu Guo , Beijing University of Technology; Thomas Bieler, Michigan State University; Andre Lee, Michigan State University; Rajen Sidhu , Intel Corporation

Wednesday AM Room: 204
February 17, 2010 Location: Washington State Convention Center

Session Chairs: Iver Anderson, Iowa State University; Jenn-Ming Song, National Dong Hwa University

8:30 AM Invited
Shock Resistant and Thermally Reliable Low Ag SAC Solders Doped with Mn or Ce: *Ning-Cheng Lee*[1]; Weiping Liu[1]; Adriana Porras[2]; Min Ding[2]; Anthony Gallagher[3]; Austin Huang[4]; Scott Chen[4]; Jeffrey ChangBing Lee[5]; [1]Indium Corporation; [2]Freescale Semiconductor; [3]Motorola Inc; [4]Advanced Semiconductor Engineering Group; [5]IST-Integrated Service Technology Inc

The reliabilities of low Ag SAC alloys doped with Mn or Ce were evaluated under JEDEC drop, dynamic bending, thermal cycling, and cyclic bending test conditions against eutectic SnPb, SAC105, and SAC305 alloys. The Mn or Ce doped low cost SAC105 alloys achieved a higher drop test and dynamic bending test reliability than SAC105 and SAC305, and exceeded SnPb for some test conditions. More significantly, being a slightly doped SAC105, both SACM and SACC matched SAC305 in thermal cycling performance. In other words, the low cost SACM and SACC achieved a better drop test performance than the low Ag SAC alloys plus the desired thermal cycling reliability of high Ag SAC alloys. The mechanism for high drop performance and high thermal cycling reliability can be attributed to a stabilized microstructure,with uniform distribution of fine IMC paricles, presumably through the inclusion of Mn or Ce in the IMC.

8:55 AM
Effects of Co Addition upon Sn-8.8Zn/Cu and Sn-57Bi/Cu Interfacial Reactions: *Yu-chih Huang*[1]; Sinn-wen Chen[1]; [1]National Tsing Hua University

Eutectic Sn-Zn and Sn-Bi alloys are promising Pb-free solders, and Cu is commonly used in electronic products. Interfacial reactions between Cu substrate and Sn-Zn and Sn-Bi solders are investigated at 230 and 160°C. Two different sizes of solders, 2mg and 2g, added with different amounts of Co (up to 0.5%) are examined. The reaction products in the couples prepared with the two kinds of solders are not changed with the addition of Co, and they are γ-Cu5Zn8 and η-Cu6Sn5 phases, respectively. With and without Co addition, the γ-Cu5Zn8 phase in the Sn-Zn-(Co)/Cu couple is layer structure, and it is found that the growth rate of γ-Cu5Zn8 phase decreases with higher Co addition and smaller sizes of joints. On the other hand, the morphology of η-Cu6Sn5 phase becomes porous with the Co addition. The growth rate of η-Cu6Sn5 increases with higher Co addition, but it decreases with smaller sizes of joints.

9:10 AM
High-Temperature Lead-Free Solder Alternatives: Possibilities and Properties: *Vivek Chidambaram*[1]; John Hald[1]; Jesper Hattel[1]; [1]Technical University of Denmark

High-temperature solders have been widely used as joining materials to provide stable interconnections that resist a severe thermal environment and also to facilitate the drive for miniaturization. High-lead containing solders have been commonly used as high-temperature solders. The development of high-temperature lead-free solders has become an important issue for both the electronics and automobile industries because of the health and environmental concerns associated with lead usage. Unfortunately, limited choices are available as high-temperature lead-free solders. This work outlines the criteria for the evaluation of a new high-temperature lead-free solder material. Furthermore, a list of potential high-temperature lead-free solder alternatives has been proposed. The high-temperature stability of microstructures and mechanical properties of these potential candidate alloys have been extensively reported. Focus has also been given to the property of corrosion resistance. This paper presents the superior characteristics as well as some drawbacks of the various high-temperature lead-free solder alternatives.

9:25 AM
Improvement of Wettability and Thermal Properties at Bi Based Alloys: *Minoru Ueshima*[1]; [1]Senju Metal Industry

There is Bi based alloy as candidate to replace Pb-rich alloy because of the high melting point, but Bi is hard to get wet with Cupper electrode becase it doesn't form any intermetalic compound with Cupper. We try to improve the wetting properies of Bi on Cu by addition of small amount of Sn and In. Increase of Sn and In at Bi alloys make the wettability on Cu better, but however the soldius line of the alloys decrease to be 139 centigrade degree. It was found that the additoin of Cu and Ag is effective to restrict decreasing the solidus line. In this study, the wetting properties of Bi-xSn and Bi-xIn alloys (x=0.5,1,3,6) on Cu electrode are researched and the soldering process to restrict the decrease of the solidus line at Bi-Sn-Cu alloy is proposed.

9:40 AM
Liquid Phase Sintered Solders as Thermal Interface Materials for Conventional and High Temperature Electronic Applications: *Jia Liu*[1]; Paul Rottmann[1]; Shouvik Dutta[1]; Chelliah Nagaraj[2]; Praveen Kumar[1]; Mukul Renavikar[3]; Rishi Raj[2]; Indranath Dutta[1]; [1]Washington State University; [2]University of Colorado; [3]Intel Corp.

Liquid phase sintering (LPS) is utilized to design novel composite solder microstructures for next generation thermal interface material (TIM) applications for high power density devices. Cu-In composites are explored for microelectronic applications (up to 125°C), while Cu-Bi is studied for high temperature power electronics applications (above 270°C). The new LPS solders constitute a majority high melting phase (HMP) in a matrix of a minority low melting phase (LMP), and proffers high conductivity in conjunction with high mechanical compliance. The Cu-In system is susceptible to the formation of interfacial intermetallics, the effects of which on the evolution of sintered density and properties is discussed. The Cu-Bi system is less thermally conductive, but is highly mechanically compliant above the melting point of Bi, making it very attractive as a 'thermal grease' TIM. The mechanical and thermal properties of LPS solder systems with and without LMP melting will be discussed in detail.

9:55 AM
Development of Sn-Ag-Cu-X Alloys for Electronic Assembly: *Adam Boesenberg*[1]; Iver Anderson[2]; Joel Harringa[2]; [1]Iowa State University; [2]Ames Laboratory of US DOE

The global electronic assembly community is striving for a robust replacement for Pb-containing solders due to increased environmental regulations. A family of Pb-free ternary solder alloys based on Sn-Ag-Cu (SAC) compositions has shown promise for implementation; but issues in reliability in certain assembly and operating environments have arisen. Elemental (X) additions (Co, Ni, Mn, Zn, Al, Fe) to SAC3595 were analyzed for better understanding of heterogeneous nucleation mechanisms for greater control in joint solidification. Solderability on Cu of down-selected SAC+X alloys (Mn, Zn, Al) was tested using micro-wetting globual testing due to concern about increased oxidation during the reflow process. Minimization of the X concentration was investigated in simplified Cu joints by differential scanning calorimetry and joint microstructure analysis to determine undercooling effects and solidification morphology on single and multiple reflow cycles. Supported by Iowa State University Research Foundation and Nihon-Superior, Inc., through Ames Lab contract No. DE-AC02-07CH11358.

10:10 AM Break

10:25 AM
On the Mechanism of Retarding Cu3Sn Growth by Ni Addition: *Yi-Wun Wang*[1]; C. Robert Kao[1]; [1]National Taiwan University

The effect of Ni addition to solders reacting with Cu was investigated in order to understand the mechanism of retarding Cu3Sn growth. The liquid-solid reaction and solid-state annealing behavior of two high-lead solders, 90Pb10Sn-xNi and 95Pb5Sn-xNi (x=0~0.1 wt.%), was examined. The reflow temperature and time are 350°C and 2 min. The samples were then subjected to solid-state aging at 160°C for 500, 1000 and 2000 hrs. After reflow, Cu3Sn formed on the Cu substrate for both solders. However, solid-state annealing produced significantly different reaction products for the two solder compositions. In the case of 90Pb10Sn solder, the Cu3Sn and Cu6Sn5 grow after 160°C aging. On the other hand, in the case of 95Pb5Sn solder, only Cu3Sn continued to grow after 160°C aging. The experimental results show that the Ni addition to high-lead solder doesn't retard Cu3Sn growth. Ni retards the growth of Cu3Sn through Cu6Sn5.

10:40 AM
On the Merits of Transient Liquid Phase Bonding as a Substitute for Soldering with High-Pb Alloys: *Alexandre Kodentsov*[1]; [1]Eindhoven University of Technology

There is still no obvious replacement for high-lead solder alloys that are in the use today for electronics assembly operations.Experimental and theoretical studies conducted in the framework of the European COST Action MP0602 established two practical routes in which further effort to find a suitable no-lead replacement should be directed. One is to design solders that contain no lead, like Zn-Al and/or Bi-Ag based (near-) eutectic alloys. The other option is to find substitute joining technologies for traditional soldering. It is possible to develop a cost-effective Transient Liquid Phase (TLP) joining process for the fabrication of high-temperature Pb-free interconnections. Through the judicious selection of Sn- or Bi-based interlayer between under bump metallization and substrate pad, transient liquid-phase bonding can be achieved at ~240 or ~270 C, and the resulting joints are capable of service at elevated temperatures.

10:55 AM
Thermal, Mechanical Stability, and Wetting Behavior of Novel Cerium (Ce)-Containing Pb-Free Solders on Cu and Ni-Au Metallization: *Huxiao Xie*[1]; Ling Jiang[1]; Mukul Renavikar[2]; Nik Chawla[1]; [1]Arizona State University, School of Mechanical, Aerospace, Chemical, and Materials Engineering; [2]Intel/ATTD

Traditional Pb-free solders such as Sn-Ag-Cu (SAC) show relatively low ductility and poor damage tolerance. Our research has shown that SAC-alloy doped with trace amounts of Ce exhibits a substantial improvement in ductility, with a relatively small decrease in strength. These alloys also have better oxidation resistance than other rare earth-containing solders such Lanthanum and Yttrium. In addition to the beneficial bulk and surface properties, it is imperative to understand the long-term thermal and mechanical stability as well as the interaction of Ce-containing SAC solders with most prevalent surface metallizations. As a consequence, microstructural characterization, as well as shear strength of SAC305 and SAC-Ce (0.5 wt. %) on Cu and electroless Ni-Au metallizations were studied in the as-processed and thermally aged conditions. The wetting behavior of SAC and SAC-Ce on Cu was evaluated by measuring the contact angle and spreading area ratio on underlying metallizations.

11:10 AM
Polymers Investigation for 3D IC Stacking Technology: Cheng-Ta Ko[1]; Wei-Chung Lo[1]; *Kuan-Neng Chen*[2]; Huan-Chun Fu[1]; Zhi-Cheng Hsiao[1]; Yu-Hua Chen[1]; [1]Industrial Technology Research Institute; [2]National Chiao Tung University

3D IC has been generally acknowledged as the next generation semiconductor technology with the advantages of small form factor, high performance, low power consumption, and high density integration etc. The stacked bonding is one of the core technologies to perform 3D interconnection. One emerging approach with high yield and reliability is hybrid bonding, which can achieve interconnection with adhesive serving reinforcement of the mechanical stability between stacked ICs. To develop the metal/adhesive hybrid bonding technology, several polymer materials were evaluated as the adhesive in this research. The material has to basically possess high thermal resistance for well collocation with metal bonding. Analyses such as SAT and shear test were adopted to evidence the bonding condition and strength. Samples with hybrid scheme were fabricated to perform hybrid bonding and realize the compatibility in whole process. The process conditions and evaluation results of material candidates will be disclosed in the paper.

11:25 AM
Modeling of Reflow Temperatures and Wettability in Lead-Free Solder Alloys Using Hybrid Evolutionary Algorithms: *Chedtha Puncreobutr*[1]; Gobboon Lohthongkum[2]; Prabhas Chongstitvattana[1]; Boonrat Lohwongwatana[2]; [1]Department of Computer Engineering, Faculty of Engineering, Chulalongkorn University; [2]Department of Metallurgical Engineering, Faculty of Engineering, Chulalongkorn University

When designing new solder alloys, many key performance properties must be considered and optimized, for example, liquidus and solidus temperatures, the reflow-ability, the strength of soldered contacts, wettability and microstructural stability, etc. With more parameters, the optimization process becomes complex and tedious. Hybrid evolutionary algorithms model is proposed as a tool for designing new alloy compositions by optimizing three key aspects: wettability, liquidus and solidus temperatures. The first aspect was investigated using Butler's equation. The liquidus and solidus of Sn-Ag-Cu-Bi-In solders were investigated using CALPHAD. The results were used as training database for genetic programming, an evolutionary algorithm which mimics nature by allowing only superior genetic traits to survive. With three key objectives combined, genetic algorithm was used to identify worthy candidates. Experimental results confirmed that the algorithms were reliable. The model can be extended to other key performance parameters to produce a complete assessment of optimized alloy recipes.

11:40 AM
Effects of Processing and Amount of Co Addition on Shear Strength and Microstructural Development in Sn-3.0Ag-0.5Cu Solder Joint: *Limin Ma*[1]; Feng Tai[1]; Guangchen Xu[1]; Fu Guo[1]; [1]Beijing University of Technology

Co has been considered as one of the promising alloying elements to improve the strength and reliability of Pb-free solders, due to its high modulus values and good bonding with Sn. The characteristic microstructure and mechanical properties of Sn-3.0Ag-0.5Cu+XCo (X=0, 0.1, 0.2, 0.45 and 1.0 wt. %) solder joint with Cu substrate were investigated. This study was attempted to clarify the effects of different weight fraction of Co addition on solder joint. The change of undercooling degrees and solidifying phases of solder joints were investigated. An exploration of different solder joint fabrication methods, with both solder preforms and solder paste, was also carried out. The interfacial intermetallics layer stability and stress strength of the solder joints were systematically studied and compared with the control samples. The change in mechanical integrity of the solder joints were correlated with the microconstituents in the solidified solder joints.

Polymer Nanocomposites: Carbon Fibers and Carbon Nanotubes

Sponsored by: The Minerals, Metals and Materials Society
Program Organizer: John Zhanhu Guo, Lamar University

Wednesday AM February 17, 2010
Room: 309
Location: Washington State Convention Center

Session Chairs: John Zhanhu Guo, Lamar University; Carla Leer, Applied Sciences, Inc

8:30 AM Introductory Comments

8:35 AM Keynote
An Assessment of the Science and Technology of Carbon Nanotube Composites: *Tsu-Wei Chou*[1]; Erik Thostenson[1]; Limin Gao[1]; [1]University of Delaware

This paper examines the recent advancements in the science and technology of carbon nanotube (CNT)-based fibers and composites. The assessment is made according to the hierarchical structural levels of CNTs used in composites, ranging from 1-D to 2-D to 3-D. At the 1-D level, fibers composed of pure CNTs or CNTs embedded in a polymeric matrix produced by various techniques are reviewed. At the 2-D level, the focuses are on CNT-modified advanced fibers, CNT-modified interlaminar surfaces and highly oriented CNTs in planar form. At the 3-D level, we examine the mechanical and physical properties CNT/polymer composites, CNT-based damage sensing, and textile assemblies of CNTs. The opportunities and challenges in basic research at these hierarchical levels have been discussed.

9:15 AM

Hierarchical Nanocomposites Based on Controlled CNT Arrays: *Wei Chen*[1]; Steven Nutt[1]; [1]University of Southern California

The CVD growth of carbon nanotube arrays with controlled diameter, density, and length on carbon fibers was attained through a freeze-dry assisted catalyst deposition method in this study. Preheating temperature and catalytic solution concentration were proven to be the key parameters in determining CNT diameter and forest density respectively. The hierarchical nano-structure was incorporated into an epoxy matrix through a vacuum bag process and characterized for thermal and mechanical performances.

9:35 AM Invited

Study on Damping Properties of Polyetherimide/Graphite Nano-Platelet Composites: *Anthony Perugini*[1]; Bin Li[1]; Weihong Zhong[1]; [1]Washington state university

Polyetherimide (PEI)/graphite nano-platelet (GNP, both as-received and chemically treated) composites with 0.5wt% to 3.0wt% GNPs were prepared for damping applications in aerospace structures. The influences of concentration, size, as well as chemical surface treatment of the GNP, on damping properties of the composites, were studied by dynamic mechanical property analyzer. The results show that, the storage modulus of PEI/GNP composites was noticeably improved with only 0.5 wt% GNP loading. The addition of as-received GNPs did not show obvious impact on the energy dissipation of the composites. To improve the interfacial interaction, chemical surface treatments of GNPs were carried out using a silanization method, which could greatly improve the damping properties of the PEI/GNP composites due to the enhanced frictional motion between PEI molecule chains and GNPs, as well as between the interlayers.

9:55 AM

Mechanomutable Carbon Nanotube Arrays: *Markus Buehler*[1]; Steven Cranford[1]; [1]Massachusetts Institute of Technology

Here we present atomistic-based multi-scale simulation studies of a magnetically active array of carbon nanotubes to illustrate the concept of mechanomutability. We show that applying external fields, it is possible to change the nanostructure and to induce a desired mechanical response. Direct numerical simulations are reported that illustrate this concept via mechanical testing through nanoindentation. Specifically, the contact stiffness of an array of carbon nanotubes can be changed reversibly from approximately 73 MPa to 910 MPa due to the application of an external field. A hierarchical approach, implemented through coarse grain molecular modeling, is utilized dto develop a framework that can successfully collaborate atomistic theory and simulations with material synthesis and physical experimentation, and facilitate the progress of novel mechanomutable structural materials. Further studies of mutable polymer nanotube arrays are presented, and a comparison with experimental results is discussed.

10:15 AM Break

10:45 AM Invited

Plasma Coating and Magnetic Alignment of Carbon Nanotubes in Polymer Composites: *Donglu Shi*[1]; Hoon Sung Cho[1]; Christopher Huth[1]; Jie Lian[2]; [1]University of Cincinnati; [2]Rensselaer Polytechnic Institute

Carbon nanotubes were modified by a novel plasma polymerization method. In this process, ultrathin films of polystyrene were deposited on the surfaces of carbon nanotubes for improved dispersion. A small percent by weight of these surface-coated nanotubes were incorporated into polystyrene to form a polymer nanocomposite. The plasma coating greatly enhanced the interfacial bonding in the polymer matrix. High-resolution transmission-electron-microscopy images revealed an extremely thin film of the polymer layer (~3 nm) at the interface between the nanotubes and matrix. Tensile test results showed considerably increased strength in the coated nanotubes composite while an adverse effect was observed in the uncoated composites. Furthermore, the carbon nanotubes were magnetically aligned in the polymer composites, responsible for a pronounced anisotropy in mechanical strength. The processing details and mechanical properties of the carbon nanotube composites will be presented.

11:15 AM Invited

Interfacial Interaction among Carbon Nanofibers Reinforced Epoxy Nanocomposites: *Jiahua Zhu*[1]; Suying Wei[1]; John Zhanhu Guo[1]; [1]Lamar University

Surface functionalized carbon nanofibers (s-CNFs) and as-received CNFs (u-CNFs) with different loadings were dispersed in epoxy monomers, and the rheological and electrical properties were comparatively investigated at different oscillatory frequencies and temperatures. CNFs network structure was formed once the loading exceeds the percolation point, which can be characterized by the change of storage modulus and loss modulus. Results show that the percolation points are strongly related to the surface character of the CNFs, and also the CNFs loading corresponding to the sharp increase of electrical property are found to be well consistent with the rheological percolations. In bulk matrixes, the interfacial strength between the s-CNFs and solid matrixes were greatly improved owing to the covalent bonding arising from the attached amine group on s-CNFs surface and epoxy monomers. Thus, the mechanical and thermal properties are significantly enhanced as compared to the u-CNFs/epoxy nanocomposites. The reinforcing mechanisms are proposed.

11:45 AM

Localized Characterization of Carbon Nanotubes and Carbon Nanotube Reinforced Nanocomposites Using Novel Micromechanical Devices: *Yogi Ganesan*[1]; Yang Lu[1]; Cheng Peng[1]; Hao Lu[1]; Roberto Ballarini[1]; Boris Yakobson[1]; Jun Lou[1]; [1]Rice University

The knowledge of carbon nanotube (CNT) strength and the fundamental mechanisms that govern mechanical behavior at the nanotube-matrix interface are critical for CNT reinforced nanocomposite development i.e. in order to realize the theoretically and computationally predicted potential of CNTs as reinforcements for high performance composites. In this work, we have developed a simple micro-fabricated device that could be used within an SEM/TEM chamber in order to perform in situ tensile tests of individual CNTs treated with different functional groups and nanoscale CNT pullout experiments using different matrices quantitatively. The insights gained from this research could potentially help engineer superior CNT reinforced nanocomposites by enabling the development of powerful predictive models.

12:05 PM

Quantification of Carbon Nanotube Distribution and Property Correlation in Nanocomposites: *Srinivasa Bakshi*[1]; Ruben Batista[1]; Arvind Agarwal[1]; [1]Florida International University

Quantification of the quality of distribution is essential in carbon nanotube (CNT) composites since it reflects the homogeneity of the properties. In this work, an attempt is made to quantify the quality of distribution of carbon nanotubes in a metal matrix composite by two methods. Two parameters have been proposed which are complimentary. The first one called Dispersion Parameter (DP) is based on the image analysis technique and is obtained based on the size of CNT cluster while the second one, named the Clustering Parameter (CP) is based on distances between centers of the nanotubes obtained by Delaunay triangulation. The method is applied to compare the distribution of nanotubes in three micrographs of CNT reinforced aluminum composite. A comparison between two quantification techniques is made. Carbon nanotube distribution obtained by image analysis technique is utilized to correlate and account for experimentally obtained elastic modulus values of the nanocomposite by nanoindentation.

Processing Materials for Properties: Functional Materials Processing

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division
Program Organizers: Brajendra Mishra, Colorado School of Mines; Akio Fuwa, Waseda University; Paritud Bhandhubanyong, National Metal and Materials Technology Center

Wednesday AM — Room: 617
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Sreeramamurthy Ankem, University of Maryland; Vikas Sinha, UES, Inc.

8:30 AM Keynote
Melting Behavior of Solid Particles during High Temperature Bath Processing: *Florian Kongoli*[1]; Ian McBow[1]; E. O'Brien[1]; S. Llubani[1]; [1]FLOGEN Technologies Inc

In primary smelting as well as in recycling processes the solid remaining materials from several processing units or crashed electronic materials are recycled in order to extract their valuable residual elements. In some actual processes the recycling is done by simply feeding the solid particles into a furnace while the injection of these particles into a bath is also a viable opportunity. In this paper the melting behavior of the slag particles in recycling processes is quantified through an original non-equilibrium physical model that takes into account all the factors that influence the melting behavior of the solid particles such as the slag particle size, temperature, chemical composition and physical properties of both the slag particles and that of the furnace bath as well other physical parameters. The advantages of this physical model related to the increase of efficiency and productivity of these recycling processes are also discussed.

9:00 AM
Direct Reversal Imprint Lithography of Indium-Tin Oxide (ITO) Nanoparticles for Improvement of Light Extraction Efficiency of GaN Based LED Devices: *Ki-Yeon Yang*[1]; Sang-Chul Oh[1]; Kyeong-Jae Byeon[1]; Heon Lee[1]; [1]Korea University

Recently, light emitting diodes (LEDs) has widely used as a light source for LCD back-light, mobile display, indoor lighting source due to low power consumption, long lifetime and thin configuration. In order to develop the highly efficiency GaN based LED devices, a number of researches have been progressed for enhancement of its low light extraction efficiency. For making the most enhancement of light extraction efficiency and applying into industrial process, photonic crystal patterns must be formed by simple process with low process cost. In this study, indium-tin oxide (ITO) nanoparticle (NP) photonic crystal patterns were formed on the ITO/GaN based blue LED substrate by direct reversal imprint lithography. And we confirmed that light extraction efficiency of GaN based blue LED with ITO NP photonic crystal patterns was drastically enhanced in relation to that of the LED without ITO NP photonic crystal patterns through analysis of photo-luminescence and electro-luminescence.

9:20 AM
Fabrication of Photonic Crystal Patterns on GaN-Based Light-Emitting Diodes to Improve Photon Extraction Efficiency: *Kyeong-Jae Byeon*[1]; Eun-Ju Hong[1]; Hyoungwon Park[1]; Kyung-Min Yoon[1]; Joong Yeon Cho[1]; Heon Lee[1]; [1]Korea University

In order to enhance the light extraction of the GaN-based light-emitting diodes (LEDs), various photonic crystal patterns were formed in the LED structure by nanoimprint lithography. Indium tin oxide electrode and p-GaN top cladding layer were patterned with photonic crystals by UV imprinting and dry etching process. Photonic crystal patterns could be uniformly formed on 2 inch whole LED substrate by using a flexible polymer stamp, which can ensure conformal contact between the stamp and LED wafer, during imprinting process. As a result, photoluminescence intensity of the patterned LED was drastically increased by prominent light scattering and light coupling with photonic crystal patterns. And electroluminescence intensity of the patterned LED device was enhanced up to 25% compared to that of the non-patterned LED device. By measuring I-V characteristics of the patterned LED and non-patterned LED devices, electric degradation was analyzed.

9:40 AM
Indium-Gallium-Zinc-Oxide Based Thin-Film-Transistor for Display Devices.: Sonachand Adhikari[1]; Rajeev Gupta[1]; *Deepak*[1]; Ashish Garg[1]; [1]Indian Institute of Technology Kanpur

Indium-Gallium-Zinc-Oxide (IGZO), which exhibits higher carrier mobility than a-Si, is more suitable for thin film transistors in backplane of active-matrix flat panel displays. IGZO films deposited by pulsed laser deposition (PLD) or sputtering require preparation of a target by mixing individual oxides and sintering them. Because this process is not yet standardized, considerable variation in optimal composition is reported in literature. We have mixed the three oxides and sintered them under different temperature, time and processing conditions. Based on detailed X-ray diffraction analysis and comparing it with compositional analysis by wet and dry methods, we determined the conditions in which sintering is complete. Using the target thus made, films deposited by PLD under partial pressure of oxygen varying between 10^{-2} - 10^{-5} mbar are characterized for transparency and conductivity. We believe, the variation reported in literature for IGZO composition may be due to inadequate method of preparing the target.

10:00 AM
Production and Characterization of ASTM F75 Balls Produced by the Uniform-Droplet Spray Process: *Sudesna Roy*[1]; Teiichi Ando[1]; [1]Northeastern University

Mono-size droplets of a Co-28wt.%Cr-5wt.%Mo alloy (ASTM F75) were produced by the uniform-droplet spray (UDS) process, a capillary jet breakup process, in diameters ranging from 300 μm to 700 μm, and characterized for their solidification microstructures. The 700 μm droplets all had a well-developed dendritic microstructure, while the 300 μm droplets exhibited a microcrystalline microstructure, indicative of dendrite fragmentation, which may take place during the post-recalescence plateau stage. Conditions for dendrite fragmentation, determined with a dendrite fragmentation model and recently developed simulations models for the nucleation and crystallization kinetics of traveling molten droplets, also suggest the occurrence of dendrite fragmentation in the 300 μm.

10:20 AM Break

10:30 AM
Preparation and Characterization of Microfibrous Entrapped Solid Adsorbents for Desulfurization of Liquid Fuels: *David Cocke*[1]; Mohammad Islam[1]; Jewel Gomes[1]; Eric Peterson[2]; Morgan Reed[1]; Doanh Tran[1]; Hylton McWhinney[3]; [1]Lamar University; [2]Fluor; [3]Prairie View A&M University

Existing hydrodesulfurization technologies are not competent to reduce the sulfur content of gasoline or diesel to less than 10 ppmw, partly because remaining sulfur compounds in current commercial liquid fuels are thiophenic sulfur compounds. Even if the severity of the reaction is increased at high H2 presssure and high temperature, it is difficult to reach sulfur removal below 5 ppmw while the olefin content in the fuel is kept unchanged. In this study, we focused on preparation of microfibrous entrapped alumina support particles by impregnation method such as microfibrous entrapped Zn/Al2O3 for desulfurization. As microfibrous agent, glass and silica were used. The structure and the morphology of the porous materials were characterized by XRD, SEM/EDS, XPS, and TGA.The analysis of the porous structure was justified using BET equations, H–K equation and BJH theory, and its physicochemical behaviors was compared with traditional Zn/Al2O3 catalysts.

10:50 AM
Energy Efficient Sintering of Al/Cu Nanocomposites Using Different Microwave Power Levels: *Shashank Nawathe*[1]; W.L.E. Wong[2]; M. Gupta[2]; [1]University of California, Berkeley; [2]National University of Singapore

Pure aluminum and Al/Cu nanocomposites were fabricated by integrating pure aluminum with nano copper reinforcement using powder metallurgy route incorporating energy efficient microwave assisted rapid sintering technique. The composites were subjected to different microwave power levels during the sintering. Microstructural characterization studies revealed the presence of minimal porosity and reasonably uniform distribution of the reinforcement in the nanocomposites. Mechanical characterization revealed that the maximum strength is achieved for composite sintered at 50% power level while the highest ductility is achieved for composite sintered at 30% power level. The best overall combination of mechanical properties assessed in terms of work of fracture was realized in the composite sintered at 100% microwave power level. An attempt is made in the present study to correlate the effect of different microwave power levels on the characteristics of the Al/Cu nanocomposites.

11:10 AM
Microstructural Characterization of Shape Memory Alloys for Ferromagnetic Applications: *F. Khalid*[1]; [1]GIK Institute of Engineering Science and Technology

Ni-Mn-Ga shape memory alloys are employed for applications in actuation and sensing, robotics and aerospace industry. These alloys exhibit ferromagnetic behavior and are capable of demonstrating large reproducible strains in moderate magnetic fields. This work presents a study on the effect of annealing treatment on the microstructure and phases that are evolved in Mn-rich off-stoichiometric compositions of alloys. Microstructural and XRD results revealed martensitic structure at RT in the alloys with Mn=28at% whereas the alloy containing higher Ga (>22at%) revealed austenitic structure at room temperature. Homogenization followed by annealing treatment has shown reduction in segregation, grain growth and formation of ordered structure and consequently its influence on final properties is explained.

11:30 AM
Anisotropic Crystallization of Uniaxially Pressed Mixed Rare Earth-Iron-Boron Alloys: *Nathaniel Oster*[1]; Iver Anderson[2]; Wei Tang[2]; Yaqiao Wu[2]; Kevin Dennis[2]; Matthew Kramer[2]; R. McCallum[2]; [1]Iowa State University; [2]Ames Lab

Anisotropic nanocrystalline mixed rare earth (MRE) magnet alloy particulate for use in polymer-bonded magnets shows promise for use in high torque electric motors and other applications which require high energy density magnets capable of performing at elevated temperatures. A novel method of forming particulate with the desired microstructure from the amorphous state is presented. Due to processing differences between the proposed method and traditional methods, this technique shows promise for reduction in processing costs. In this study, amorphous MRE-iron-boron alloy particulate was uniaxially pressed during crystallization to induce texture. Texture can be formed because anisotropy in the crystal cell provides preferred growth directions under non-hydrostatic stress. Microstructure and texture are observed through transmission electron microscopy, scanning electron microscopy, and x-ray diffraction. Results will be presented. Supported by DOE-EERE-FCVT Office through Ames Lab contract DE-AC02-07CH11358

11:50 AM
The Effect of Sputtering Parameters on the Phase Formation of Sputtered Tantalum: *Anahita Navid*[1]; Andrea Hodge[1]; [1]University of Southern California

The phase transitions in magnetron sputtered Tantalum as a function of residual stress and internal plasma conditions are presented in this study. The formation of body centered cubic (BCC) and tetragonal tantalum was observed on films deposited on a Si substrate at pressures between 0.3 and 1.4 Pa. The results demonstrate the formation of BCC tantalum at a 0.7 Pa sputtering pressure at various power settings. However, any other sputtering pressure did not yield a BCC structure but rather mixed BCC/tetragonal or a tetragonal phase. The texture and residual stress of both BCC and tetragonal tantalum changed significantly with increasing pressure and film thickness. In addition, the effect of underlayer material on the corresponding phase formation will also be presented for various sputtering pressures.

12:10 PM
TiO2 Aggregates for Dye-Sensitized Solar Cells Application: *Qifeng Zhang*[1]; Xiaoyuan Zhou[1]; Christopher Dandeneau[1]; Kwangsuk Park[1]; Supan Yodyingyong[1]; Guozhong Cao[1]; [1]University of Washington

TiO2 aggregates were synthesized via a hydrolysis of alkoxide of titanium(IV) in acetic acid aqueous. The aggregates are in submicron size, feature a spherical porous structure, and consist of ~10-nm anatase TiO2 nanocrystallites. When such aggregates are used in dye-sensitized solar cells, they impart an extremely large internal surface area to the photoelectrode film for dye molecule adsorption, and meanwhile may generate effective light scattering in view of their submicron size that is comparable with the wavelengths of visible light. When compared with the traditional dye-sensitized solar cells, in which the photoelectrode film only comprises TiO2 nanoparticles, the solar cells based on TiO2 aggregates show a significant improvement in the light harvesting efficiency and, thus, contribute to the overall conversion efficiency. It is anticipated that TiO2 aggregates would have a practical application in the filed of solar cells in the future.

Recycling General Sessions: Metals

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division, TMS Light Metals Division, TMS: Recycling and Environmental Technologies Committee
Program Organizer: Joseph Pomykala, Argonne National Laboratory

Wednesday AM Room: 206
February 17, 2010 Location: Washington State Convention Center

Session Chair: Joseph Pomykala, Argonne National Laboratory

8:30 AM
Preliminary Research on Preparation Al-Si-Ti Alloy with Aluminum Ash as Electrolysis Materials: Liu Qingsheng[1]; *XUE Jilai*[2]; JING Qingxiu[1]; [1]Jiangxi University of Science and Technology; [2]University of Science and Technology Beijing

A new method of recycling aluminum ash for preparation Al-Si-Ti alloy was studied in this paper. In the experiment, first the aluminum ash was pretreated by leaching and calcining process, the fine purity and phase of the intermediate oxide powder up to electrolysis demands, then, could be obtained, which was treated by molten salt electrolysis. Finally, the Al-Si-Ti alloy was successfully obtained through electrochemical co-deposition in the cathode shows a typical as-cast microstructure. This new recycling method can produce high quality alloy and may bring remarkable economic and social benefits.

8:50 AM
Effective Utilization of Wastes Generated in the Integrated Aluminium Production - A Review: *Narasimharaghavan Krishnaswamy*[1]; Nand Kumar Kshatriya[1]; Bibhu Mishra[1]; Ramaswamy Jagannathan[1]; Durba Khasyap[1]; [1]Bharat Aluminium Co. Ltd., (A Unit of Vedanta Resources Plc.,), BALCO Nagar, Korba

The major wastes generated in the integrated Aluminium process are: Red Mud from the Bayer process, Carbon skimming, Spent Pot Lining from the Aluminium reduction process, Ash from the power plants which give energy to the reduction process and Aluminium dross from the Cast house and Foundry. In this review our recent attempts to recover caustic and the value added minerals from Red Mud, effective recovery of Fluoride salts from the carbon skimming, use of fly ash and red mud in the production of cost effective bricks for construction and our efforts towards reduction in dross generation in Cast House and Foundry has been discussed. Jarosite, the waste from the Zinc industry has been used in the recovery of value added constituents from the red mud.

9:10 AM
Stabilization of Chromium-Based Slags with MgO: Hugo Cabrera-Real[1]; *Antonio Romero-Serrano*[1]; Beatriz Zeifert[1]; Manuel Hallen-Lopez[1]; [1]IPN

This work investigated the chemical and mineralogical properties of CaO-SiO2-CrOx-CaF2-MgO slags. Synthetic slags were prepared and the effect of the slag basicity (CaO/SiO2) and MgO contents on the stability of the mineralogical species formed was analyzed. The morphology and composition of the slags were analyzed by XRD and SEM-EDS, whilst their chemical stability was evaluated by leaching with an aqueous acetic acid solution. It was found that in slags with CaO/SiO2 = 1, the main Cr-compound was MgCr2O4 spinel, which forms octahedron crystals. Small amounts of CaCr2O4 and CaCrO4 were also observed. It was found that increasing the slag basicity from 1 to 2 the compounds MgCr2O4 and CaCr2O4 were formed together with the Cr(V)-containing compound complex Ca5(CrO4)3F which forms hexagonal crystals. The results showed that the highest chromium concentration levels in the leaching liquors corresponded to slags with CaO/SiO2 = 2, probably owing to the formation of Ca5(CrO4)3F.

9:30 AM
Preparation of Potassium Ferrate by Hypochlorite Oxidation Method: Guomin Jiang[1]; *Liyuan Chai*[1]; Yunyan Wang[1]; Yude Shu[1]; Min Yue[1]; [1]Central South University

Potassium ferrate is an excellent multifunctional agent for wastewater treatment, but its preparation is crucial. The improved hypochlorite oxidation method was used to prepare potassium ferrate in this study. Iron nitrate, the preferred iron source, was added into hypochlorite solution and then the stabilization agent was added during the purification process of product. The influence of available chlorine content, iron molecular proportion, reaction temperature and reaction time on potassium ferrate preparation was investigated. The optimal condition for potassium ferrate preparation is 15% of available chlorine content,0.6 of iron molecular proportion,30° of reaction temperature,45min of reaction time. The yield of potassium ferrate is about 67% with more than 99% of purity. The structure and performances of the product was characterized by XRD,EDX, SEM, TG and IR and the results show that the prepared product is consistent with the properties of potassium ferrate(VI).

9:50 AM Break

10:00 AM
Isotherm and Kinetics Studies of the Biosorption of Cobalt from Aqueous Solutions by Waste Materials: *Chen Yunnen*[1]; Fan Jingbiao[1]; [1]Jiangxi University of Science and Technology

In the present study, waste materials like pine sawdust and spent grains were investigated to assess their potential for removal of cobalt ion from water by the process of biosorption. The effects of solution pH, reaction time and initial concentration were studied in batch experiments. The removal efficiency of Co(II) by spent grains was higher than that of pine sawdust. The initial removal was rapid and equilibrium was established in less than 90 min. Equilibrium data all agreed well with Freundlich isotherm model for the two metal-biomass sorption processes. Good correlation coefficients were obtained for the pseudo second-order kinetic model. Pine sawdust and spent grains were shown to be promising biosorbents for Co(II) removal from aqueous solutions.

10:20 AM
Novel Technology for Wastewater Treatment by Biologics in Hydrometallurgical Processes of Lead-Zinc: Qingwei Wang[1]; *Liyuan Chai*[1]; Yunyan Wang[1]; Qingzhu Li[1]; Zhihui Yang[1]; [1]Central South University

Heavy metal-containing wastewater from hydrometallurgical processes of lead-zinc was treated by biologics in a 200 m3/h industrial scale experiment. The result shows that Zn concentration declined from 50.28 mg/L~240.81 mg/L to 0.21 mg/L~1.98 mg/L, Pb from 1.00 mg/L~13.47 mg/L to 0.083 mg/L~0.71 mg/L, Cu from 0.24 mg/L~2.38 mg/L to 0.059 mg/L~0.40 mg/L, Cd from 2.12 mg/L~23.47 mg/L to 0.011 mg/L~0.071 mg/L and As from 0.50 mg/L~6.00 mg/L to 0.005 mg/L~0.10 mg/L. The concentrations of the above heavy metals in the treated water were lower than that in Integrated Wastewater Discharge Standard (GB8978~1996) in China. Furthermore, the treated wastewater was recycled and reused in smelter plant. Zinc content in hydrolytic sludge reached up to 34.04%, which indicates that this sludge can be used to recover valuable metals.

10:40 AM
Study on the In-Situ Remediation of Cr-Contaminated Soil by Indigenous Microorganism: *Shunhong Huang*[1]; [1]Hunan Research Institute of Nonferrous Metals, Changsha

Based on the optimization of culture medium composition and growth conditions and ability of Cr(VI) reduction, the bioremediation of Cr-contaminated soil can be achieved by adding culture medium in soils to stimulate the activity of indigenous microorganism. The optimal condition for the Cr(VI) reduction by indigenous microorganism was 5g glucose and 5g yeast extract per kg soil at 30°C and the ratio of soil and water was 1:1. Under the optimal condition, 92% of total Cr(VI) in soil contaminated by chromium-containing slag heap was removed and water soluble Cr(VI) was completely removed at 4 days.

11:00 AM
The Optimum Condition for Cr(VI) Bioremediation in Soils Contaminated by Chromate Ore Processing Residue: Changqing Su[1]; *Yonghua Zhu*[1]; Bing Wang[1]; Hangbin Li[1]; Yingping Liao[1]; [1]Central South University

A batch incubation experiment has been carried out to investigate the optimal condition for the microbial remediation of hexavalent chromium (Cr(VI)) in soils contaminated by chromate ore processing residue (COPR) at Hunan Iron-Alloy Factory in China. The results indicated that glucose and yeast extract was the optimal component of culture medium and the quantities of the above components were 8 g L-1 and 13 g L-1, respectively. The favorable temperature and pH value were 30° and 10.0, respectively. A bioreactor was operated under the optimal condition and water soluble Cr(VI) in soils was reduced from 313 mg kg-1 Cr(VI) of the initial concentration to below detection limit after 30 h. Thus, there is a large potential to accomplish Cr(VI) bioremediation at the presence of indigenous bacteria by the addition of optimal culture medium in soils contaminated by chromate ore processing residue.

11:20 AM
Thermodynamic Equilibrium of Hydroxyl Complex Ions in Mn2+-H2O System: Fei Pei[1]; *Yunyan Wang*[1]; Liyuan Chai[1]; [1]Central South University

Pc-pH diagrams and -lnγ±MnSO4-I relationship for activity coefficient and ionic strength of Mn2+-H2O system have been drawn based on the thermodynamic principle of coordination chemistry combined with the Pitzer theory at 298.15K. The diagram of -lnγ±MnSO4-I indicated that -lnγ±MnSO4 increased from 0 up to 1.2147 when I changed from 0 to 0.09, increase of -lnγ±MnSO4 became slowly when I was at 1.00 -1.69, and -lnγ±MnSO4 kept constant when I was at 2.25-4.00. Diagrams of pc-pH illustrated that the minimum solubility of Mn(OH)2(s) increased with I, the pc decreased from 6.5 to 5.5 when I changed from 0 to 4.00; The pH value of the minimum solubility of Mn(OH)2(s) increased from 11.80 to 12.76 when I changed from 0 to 2.89, and pH kept constant with I increasing when I was less than 4.0. There is a simple relationship between the minimum solubility of Mn(OH)2(s) and pH in different I.

Sustainable Materials Processing and Production: Sustainable Technologies I

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division, TMS Light Metals Division, TMS: Recycling and Environmental Technologies Committee, TMS: Education Committee
Program Organizers: Christina Meskers, Umicore; Randolph Kirchain, Massachusetts Institute of Technology; Diana A. Lados, Worcester Polytechnic Institute; Markus Reuter, Ausmelt Limited

Wednesday AM — Room: 2B
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Randolph Kirchain, Massachusetts Institute of Technology; Gabrielle Gaustad, Rochester Institute of Technology

8:30 AM Introductory Comments

8:35 AM Keynote
IT and Sustainability: The Power to Transform: *Joe Johnson*[1]; [1]Cisco Systems, Inc.

The global footprint of the IT sector is estimated to be 2% of worldwide carbon emissions and growing. At the same time, innovative applications of IT have the potential to reduce global emissions many times over this amount. Recent trends, such as broad adoption of video teleconferencing technologies and virtual collaboration tools have validated IT can reduce emissions from other sectors. Opportunities such as smart grids, smart buildings and connected cities aim to apply intelligent networks to manage and reduce energy consumption on a global scale. IT products are also subject to materials restrictions and other eco-regulations which mitigate impacts by shifting environmental focus from production to products. This presentation will review these topics and the transformational capacity of IT to help achieve a sustainable future.

9:00 AM Invited
'Slag Valorisation', as an Example of High Temperature Industrial Ecology: *Daneel Geysen*[1]; Peter Jones[1]; Arnout Sander[2]; Yiannis Pontikes[1]; Özlem Cizer[3]; Tom Van Gerven[4]; Marc Craps[5]; Johan Eyckmans[5]; Bart Blanpain[1]; [1]MTM KULeuven; [2]InsPyro; [3]BWK, KULeuven; [4]CIT KULeuven; [5]HUB

Better slag valorisation is part of improving the sustainability of steel, stainless steel and non-ferrous metal production. Besides, it can improve the sustainability of other products and production processes as well. Several slag valorisation routes were studied in the past but not much high value applications are implemented yet due to technical, environmental or economic constraints. Granulated Blast furnace steel slag (GBFS) is already used for long in cement production. Its application is very successful. GBFS helps to reduce the CO_2 emissions of the cement production process. Also other slag types have potential but its quality needs to be improved by slightly optimising the metallurgical process. Besides cement, slags can be used in high quality aggregates, slag wool insulation, ceramics and carbon sincs. The paper discusses slag valorisation opportunities for different slag types and indicates non-technical limitations and opportunities such as market structures and environmental constraints and benefits.

9:25 AM

Sustainability Study in Selective Laser Sintering – An Energy Perspective: *Rameshwar Sreenivasan*[1]; David Bourell[1]; [1]The University of Texas at Austin

Additive Manufacturing (AM) processes which include Selective Laser Sintering (SLS) have experienced tremendous growth and development since their introduction over 20 years ago. Characteristic of AM processes is the creation of parts without the use of part-specific tooling. In this study, a sustainability analysis was performed on the SLS process with Nylon-12 using the Environmental and Resource Management Data (ERMD) known as Eco-Indicators. The energy perspective alone was considered and a Total Energy Indicator (TEI) value was calculated using various parameters to quantify process sustainability: process productivity, energy consumption rate, etc. A comparison of TEI values between SLS and other AM processes was made to evaluate sustainability of AM from a broad perspective.

9:50 AM Invited

***2010 Vittorio de Nora Award Winner:* Designing Crushing and Grinding Circuits for Improved Energy Efficiency**: *Zeljka Pokrajcic*[1]; [1]WorleyParsons Services Pty Ltd – Minerals and Metals

Crushing and grinding, or comminution, circuits are the most energy intensive process of a mineral processing plant. Comminution involves the physical size reduction of an orebody to a particle size sufficient for recovery of the mineral values. However, the comminution process remains inherently inefficient. The inefficiency is a result of the operating nature of comminution devices such as grinding mills, where transfer of energy between grinding media and particles in unconstrained and completely random. New comminution circuit design strategies are presented in this paper. The aim of the new strategies is to improve the overall efficiency of the comminution process and reduce the total energy consumption of a comminution circuit. This paper also explores the financial impact of certain energy efficient strategies using an analysis tool called EcoNomics™. It shows that substantial financial gains can be made by including more efficient technologies and methods in comminution circuit design.

10:15 AM Break

10:30 AM

Energy and Environmental Challenges in Aluminium Industry - A Review: *Narasimharaghavan Krishnaswamy*[1]; Bibhu Mishra[1]; Ramaswamy Jagannathan[1]; [1]Bharat Aluminium Co. Ltd., (A Unit of Vedanta Resources Plc.), BALCO Nagar, Korba

This paper discusses briefly the major reasons associated with the growth and its impact on the energy requirement and Environmental imbalance. A projection based on the present global Alumina and Aluminium requirement indicate a substantial further growth of at least 30% over the next 10 years. It is indicated that the main factors which are likely to influence investments are the environmental factors such as the Climate Change and global response to the growing energy prices and sustainable development. Each of the developed / developing nations must find response to the GHG emissions which will encourage the Aluminium Industry to make an effective contribution to global warming while preserving the international competitiveness of the industry - a challenging task. The efforts shall concentrate on improving energy efficiency in the industry possibly of the order of 25% over the next 10 to 20 years. The developments in this line are discussed.

10:55 AM

Towards Sustainable Material Usage: Investigating Limits to Secondary Aluminum Sinks: *Gabrielle Gaustad*[1]; Elsa Olivetti[2]; Randolph Kirchain[2]; [1]Rochester Institute of Technology; [2]MIT

For aluminum, substitution of primary with secondary resources decreases energy consumption; this energy advantage creates a strong economic incentive to recycle. Several authors have raised concerns that the current sinks for secondary materials may soon be saturated, impeding subsequent expansion of recycling. This work combines dynamic material flow analysis with optimal batch planning models to quantify the significance and drivers of these pending limits under several scenarios, and thereby explore potential opportunities to increase recycling. An aluminum recycling system case was developed that includes containers and packaging, automotive, and construction products and scraps. System parameters such as accumulation of tramp elements and size of dissipative scrap sinks are explored in the context of changing alloy product demand, lifetime, and collection. Insights drawn from this specific case study could be applied to multi-stakeholder, systemic models.

11:20 AM

Use of Eco Friendly Alternate Refining Flux in Aluminium Cast House - A Step towards Sustainable Development: *Narasimharaghavan Krishnaswamy*[1]; Mousumi Kar[1]; T. Prabu[1]; Charulata Mathur[1]; Gautam Dey[1]; [1]Bharat Aluminium Co. Ltd., (A Unit of Vedanta Resources Plc.,), BALCO Nagar, Korba

The major threat to the sustainability of Aluminium Industry is its significant contribution to global warming by way of generation of non eco-freiendly gasses during its production cycle from Bauxite to the finished product. Though reduction measures are taken in control and effective recovery of values from pot room gases, efforts in use of environment friendly additives in the final products production line is warrented. In this line, the present paper discribes our efforts in the use of a new generation refining flux which apart from helping in effective removal of alkali metals, reduction in inclusions and ensure a better metal cleanliness shall also aide in reduction of abnoxious gases generated during the metal refining process prior to casting. The aim of the current work was to reconcile the practical results with the old generation fluxes used. Further improvements to bring in a better metal cleanliness will also be discussed.

11:45 AM

Sustainable Electrolysis for Electrowinning and Electrorefining of Metals: *Geir Martin Haarberg*[1]; [1]Norwegian University of Science and Technology

Modern electrolysis technologies can provide possibilities for developing sustainable processes in terms of energy and environment. Laboratory experiments were carried out to study electrodeposition of iron from molten salts and aqueous solutions using an inert oxygen evolving anode to eliminate the emissions of CO_2. The possibilities of molten salt electrorefining of metallurgical grade silicon to produce solar grade silicon were also investigated. Furthermore the development of an electrochemical route using molten salts for the production of titanium is under investigation. Electrochemical techniques were used to study the electrochemical behaviour of dissolved iron, silicon, and titanium species. Bulk electrolysis was carried out to deposit pure iron, silicon, and titanium. The quality of the deposits was studied by SEM/EDS and XRD analyses.

12:10 PM Concluding Comments

The Vasek Vitek Honorary Symposium on Crystal Defects, Computational Materials Science and Applications: Grain Boundaries and Interface Structure and Properties: Joint Session with Solid-State Interfaces

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS/ASM: Computational Materials Science and Engineering Committee
Program Organizers: Mo Li, Georgia Institute of Tech; David Srolovitz, Institute for High Performance Computing, Agency for Science, Technology and Research, Singapore; Adrian Sutton, Imperial College London; Vaclav Paidar, Institute of Physics AS CR vvi; Jeff De Hosson, Univ of Groningen

Wednesday AM Room: 603
February 17, 2010 Location: Washington State Convention Center

Session Chairs: Vaclav Paidar, Institute of Physics AS CR vvi; Alan Needleman, University of North Texas; Antonia Antoniou, Georgia Institute of Technology

8:30 AM Invited
The Simulation of Grain Boundaries in Single Component and Multi-Component Systems: *Adrian Sutton*[1]; Alvin Chua[1]; Nicole Benedek[1]; Lin Chen[1]; Manuel Kurdian[1]; Sebastian von Alfthan[2]; Peter Haynes[1]; Kimmo Kaski[2]; Mike Finnis[1]; [1]Imperial College London; [2]Helsinki University of Technology

We show that the removal of atoms is an important mode of relaxation at grain boundaries in silicon and ferromagnetic iron. In silicon it is only when atoms are removed from (001) twist boundaries that new ordered configurations are obtained with lower energies than the disordered states found before. When the same thinking is applied to grain boundaries in strontium titanate we have to include in the free energy of the interface terms involving the chemical potentials of the species present. The existence of three atomic species at these boundaries increases the configurational complexity of these boundaries by astronomical factors, and the possibility of getting trapped at local energy minima is far greater than in single component systems. To overcome these problems we have developed a new computational approach based on a genetic algorithm, and we use ab initio thermodynamics to calculate the free energies.

8:55 AM Invited
Structure and Properties of Metal/Ceramic Interfaces in Materials Systems: *Manfred Ruehle*[1]; [1]MPI for Metals Research

Metal/Ceramic Interfaces (MCI) play an important, sometimes controlling, role for many materials consisting of both, metals and ceramics. The structure of MCIs as well information on bonding across the interface can be obtained by different quantitative TEM techniques. As an example, the shear strength of an MCI can be revealed by a detailed analysis of the displacement field around misfit dislocations adjacent to the MCI. Those studies were initiated by V.Vitek during his sabbatical stay in Stuttgart. (G. Gutekunst, J. Mayer, V. Vitek and M. Rühle, Phil. Mag. A 75 (1997) 1329-1355, 1357-1382) and were recently experimentally as well theoretically in a quantitative way. Results will be reported for specific, artificially grown MCIs (Ni/a-Al2O3, Cu/a-Al2O3, Pd/SrTiO3, Ni/SrTiO3).

9:20 AM Invited
Elastic and Anelastic Interface Properties in Martensitic Transformations: *Robert Pond*[1]; John Hirth[2]; [1]University of Exeter; [2]Private Individual

A model of the structure of parent-martensite interfaces has been developed based on dislocation theory. Two arrays of defects are generally present in the habit plane; one is an array of disconnections (line defects with dislocation and step character), and the other is produced by crystal defects (slip or twinning) in the martensite crystal. The object of the present paper is to discuss the elastic and anelastic properties of such defect networks. We distinguish between the plasticity induced by motion of the defect network, which is reversible or "anelastic", and the distortions arising due to the elastic fields of the defects in the static state. The former can be represented as an engineering strain expressed in terms of the Burgers vectors of the crystal defects and disconnections and their planes of motion. The latter include short-range coherency strains and small ancillary rotations that modify the orientation relationship of the crystals.

9:45 AM
Response of a Σ 11 Asymmetric Tilt Grain Boundary in Copper to an Applied Shear Stress at Finite Temperatures: *Saryu Fensin*[1]; Mark Asta[1]; Richard Hoagland[2]; [1]University of California, Davis; [2]Los Alamos National Laboratory

We present results of molecular dynamics simulations studying the temperature dependence of the structure and mechanical response to an applied shear stress for an *asymmetric* Σ 11 tilt grain boundary in copper. At higher temperatures a disordered liquid-like layer forms at the grain boundary and becomes wider in width as the melting temperature is approached from below. Upon application of shear stress the boundary undergoes incremental normal displacement also known as coupled motion at low temperatures. This behavior is analyzed to determine the atomic mechanisms of the grain boundary motion within the framework of disconnections. With increasing temperature, and associated disordering of the interface structure, the mechanical response switches to that of grain-boundary sliding at the highest temperatures, with more complex behavior being displayed at intermediate temperatures.

10:10 AM Break

10:30 AM Invited
Crystal Symmetry and Burgers-Vector Content of Grain Boundaries: *J. Cahn*[1]; Y. Mishin[2]; [1]National Institute of Standards and Technology; [2]George Mason University

Applied shear stresses can induce glissile motion of planar grain boundaries (GBs) at low temperatures similar to dislocation glide. The coupling of stress to move the GB and deform the volume it traverses depends on the GB's Burgers vector content given by the Frank-Bilby equation (FBE). Because the FBE has multiple solutions, a multiplicity of possible deformation modes and coupling factors are possible for the same GB. The complete set of coupling factors is predicted from the point symmetry of the bi-crystal and the angles which characterize the GB. The results of this analysis are compared with recent experiments and with molecular dynamics simulations.

10:55 AM Invited
Temperature Dependence of Grain Boundary Properties: *Stephen Foiles*[1]; Elizabeth Holm[1]; David Olmsted[2]; [1]Sandia National Laboratories; [2]Northeastern University

The properties of grain boundaries, such as their energy and mobilities, have been studied extensively over many years. However, the variation of these properties with temperature is still not fully explored. The temperature dependence of the interfacial free energy of a grain boundary in Ni is computed and the correlations between this temperature dependence and that of the elastic constants are explored. Some results on the temperature dependence of the boundary mobility are also presented which indicate that the variations of the mobility with temperature are substantially more complex than a simple Arrhenius type variation. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC0494AL85000.

11:20 AM
Heterophase Segregation on an Atomic Scale: Atom-Probe Tomographic Experiments and First-Principles Simulation: *David Seidman*[1]; [1]Northwestern University

In multiphase systems heterophase interfacial segregation is ubiquitous and relevant to different physical and mechanical properties of materials at both microscopic and macroscopic length scales. Heterophase interfacial segregation (or depletion) may be either monotonic (unconfined) or non-monotonic (confined): it is rare for an interface to not exhibit segregation (or depletion). We have utilized atom-probe tomography extensively to measure directly Gibbsian interfacial excesses or depletions at heterophase interfaces, using both J. W. Gibbs's and J. W. Cahn's formalisms, for a wide range of systems: nickel-based and aluminum-scandium based alloys, nickel (platinum or rhodium)/silicon interfaces, copper/magnesium oxide and silver/cadmium oxide interfaces produced by internal oxidation of dilute ternary metallic alloys. Atom-probe tomography and atom-probe field-ion microscopy are unique in their ability to measure quantitatively Gibbsian excesses with a minimum amount of data deconvolution. The experimental results are compared with first-principles calculations performed using the Vienna ab initio simulation package for nickel-based alloys.

11:35 AM
Full Delineation of Harrison's Diffusion Kinetics Regimes for Grain Boundary Diffusion: A Monte Carlo Study: *Graeme Murch*[1]; Irina Belova[1]; Thomas Fiedler[1]; [1]The University of Newcastle

Harrison's classification scheme for the kinetics regimes (A,B and C) for the measurement of grain boundary diffusivities from tracer concentration depth profiles has been very widely accepted. But the locations of the transition points between the various kinetics regimes are very poorly known thereby making detailed analysis of many grain boundary diffusion experiments quite difficult. In this paper, we make use of a recently developed Monte Carlo method that allows the determination of depth profiles in a similar way to that found in experiments. This unique approach allows the transitions between the Harrison kinetics regimes to be readily determined for various well known grain boundary models such as the parallel slab and cubic grain models. The approach is shown to be able to deal with both self-diffusion and impurity diffusion with associated segregation to grain boundaries. The complete map of the Harrison kinetics regimes will be shown.

Thermo-Mechanical Response of Molecular Solids: Multi-Resolution Theory, Simulations, and Experiments: Polymers and Composites

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division
Program Organizers: Alejandro Strachan, Purdue University; Thomas Sewell, University of Missouri-Columbia; Rodolfo Pinal, Purdue University; Chunyu Li, Purdue University

Wednesday AM	Room: 203
February 17, 2010	Location: Washington State Convention Center

Session Chair: To Be Announced

8:30 AM Introductory Comments

8:35 AM Invited
Carbon Nanotube Adhesion: Myths and Magic: *R. Pipes*[1]; [1]Purdue University

Frictionless interaction of multiwalled carbon nanotubes has been well eatablished, yet the adhesion of carbon nanotubes in bundles and arrays is a major issue in mixing and dispersion. This paper will examine the influence of CNT chirality of adhesion as measured in array flexural AFM experiments and molecular modeling simulations. These observations provide the basis for an adhesion hypothesis that suggests a strong relationship between chirality and the non-bonding adhesion of CNT in both the single and multi-walled geometries.

9:05 AM
Characterization of Material Response to Indentation Process in Composite Materials: *Harsha Yejju*[1]; Alvaro Mendoza[1]; Marisol Koslowski[1]; [1]Purdue University

The difference in bulk matrix properties of polymer and the fiber-matrix interphase region is pronounced at the nanoscale level. Here we present finite elements simulations that show the effect of the variation of the materials properties of this fiber-matrix interphase region. We carry simulations involving high density of fibers aligned in close proximity to each other. We will show the material response to indentation in the fiber-matrix interphase region with multiple fibers in close proximity to each other and the dependence of the material response on the volume of fibers and on the vicinity of the indentation probe.

9:25 AM
Microstructure Sensitive Design Framework for Elastic-Plastic Multi-Phase Materials: *Jacqueline Milhans*[1]; Dongsheng Li[1]; Hamid Garmestani[1]; [1]Georgia Institute of Technology

In this study, a microstructure sensitive design (MSD) framework for elastic-plastic properties is formulated using 2-point correlation functions. In the past, mechanical behavior predictions have been made for elastic and plastic properties in multiphase materials using correlation functions. This study extends these formulations to predict the elastic-plastic deformation behavior of composite composed by elastic and plastic materials. The formulation is based on solution of the Green's function for elastic-plastic behavior and 2-point correlation function. Material behavior is predicted by using the 2-point correlation function of a material, which characterizes the morphology and phase volume fraction of the microstructure, and the individual phase properties. These both serve as inputs to the MSD framework, which then predicts the overall behavior of the material. This methodology is applied to a glass-ceramic solid oxide fuel cell (SOFC) seal material, made up of a plastically deforming glass matrix with embedded elastic crystalline needles.

9:45 AM
Role Loading Conditions on the Mechanical Response of PMMA from Molecular Dynamics: *Eugenio Jaramillo*[1]; Alejandro Strachan[2]; [1]Texas A&M International University; [2]Purdue University

We use molecular dynamics (MD) with the DREIDING force field to characterize the mechanical response of amorphous PMMA including yield and post yield phenomena for various loading conditions. We studied periodic systems with linear dimensions 24 nm and five loading conditions: including pure shear, a series of uniaxial tension deformation with various Poisson's ratios, and isotropic expansion. We find that the pressure-modified von Mises criteria (with critical effective yield stress proportional to hydrostatic pressure) can describe our MD results accurately and with pressure sensitivity in excellent agreement with experiments. The yield stress for zero pressure obtained from MD is about 20% larger than the experimental value due to the large strain rates in the MD simulations. We also study yield criteria in terms of deviatoric and volumetric strain and find that the SIFT can describe our data accurately for deformation paths that involve significant volume expansion.

10:05 AM Invited
Multiscale Modeling of Polymer Modified Colloidal Suspensions: *Dmitry Bedrov*[1]; [1]University of Utah

We have applied a multiscale modeling approach to investigate the influence of polymer brush modifications on interactions and rheological properties in dense colloidal suspensions. Specifically, we have investigated polydispersed MgO colloidal suspensions in aqueous solutions modified with poly(ethylene oxide) brushes. The multiscale modeling approach included: a) atomistic explicit solvent molecular dynamics simulations, b) coarse-grained implicit solvent Langevin dynamics (LD) simulations, and c) coarse-grained implicit solvent implicit polymer LD simulations. Each coarse-grained model has been parametrized based on structural and thermodynamic properties obtained from the finer scale simulations.

10:35 AM Break

10:50 AM Invited
Implications of Dynamic Heterogeneity for Mechanical Behavior of Glassy Polymers: Grigori Medvedev[1]; *James Caruthers*[1]; [1]Purdue University

Existence of dynamic heterogeneities at nano-scale in glass forming materials is well established via a number of experimental techniques. However, existing models of glassy polymer relaxation do not include the dynamic heterogeneity using only the average material properties. Here we report on development of the stochastic constitutive model of glassy materials where the presence of heterogeneities is explicitly acknowledged. This effort is an initial attempt to bridge the gap between traditional molecular simulations and continuum mechanics. Two phenomena are treated: (1) the volume relaxation in response to temperature jumps (2) yield and post-yield behavior in uni-axial tension and compression. The stochastic model predicts volume behavior in a two-step "short anneal" experiment. In the uni-axial constant strain rate experiment the stochastic model predicts yield and post-yield softening and its dependence on the aging time – this is the only constitutive model to-date that predicts, rather than a priori assumes, post-yield softening.

11:20 AM Invited
Mechanical Properties of Block Copolymer Self-Assemblies: *Kim Rasmussen*[1]; [1]Los Alamos National Laboratory

We will discuss how self-consistent field theory can be applied to illuminate aspects of the mechanical properties of self-assemblies of block copolymers. Specifically, we will look at how insight into the structure of the physical crosslinking that is responsible for the mechanical properties can be obtained and correlated with observable mechanical properties. Further, we will show how self-consistent field theory methods, can provide direct calculation of the components the tensile and shear moduli that arise from structural properties of the self-assembled materials. Finally, we demonstrate how a generalized self-consistent field theory for polymer melts that explicitly includes elastic stress and strain fields can be applied to the study of block copolymers melts. This technique allows the calculation of the overall stress profile of the materials and we show that it is the result of the combined effects of chain connectivity across the interface, and the immiscible nature of the monomers.

11:50 AM
Molecular Dynamics Simulations of Crosslinked EPON862/DETDA Polymers: *Chunyu Li*[1]; Alejandro Strachan[1]; [1]Purdue University

Currently, there is a great interest in aircraft industry to use thermosetting polymers as the matrices of composites because of their higher stiffness, higher creep resistance and higher thermal resistance over thermoplastic polymers. These favorite properties come from the 3D crosslinked structures of thermosetting polymers. A fundamental understanding of the structural evolution and the relationship between material properties and molecular structures is essential. Computer simulations provide an attractive substitute technique for better understanding these polymers. The objective of this study is to provide a more comprehensive molecular dynamics (MD) simulation procedure for thermosetting polymers. The system we chose is epoxy resin EPON-862 with curing agent DETDA. In this presentation, we will systematically address the issue of atomic charge distribution and introduce a new effective charge updating approach. The procedure introduced in this paper is expected to be applied to the MD simulations of other thermosetting polymer systems without any difficulties.

12:10 PM
Role of Interface Thermal Boundary Resistance, Straining and Morphology in Thermal Conductivity of a Set of Si-Ge Superlattices and Biomimetic Si-Ge Nanocomposites: *Vikas Samvedi*[1]; Vikas Tomar[2]; [1]University of Notre Dame; [2]Purdue University

Comparison of thermal behavior of superlattices and nanocomposites considering their characteristic structural factors such as periodicity and period length for superlattices, and morphology for nanocomposites, is performed for a set of Si-Ge superlattices and Si-Ge biomimetic nanocomposites using non-equilibrium molecular dynamics (NEMD) simulations at three different temperatures (400 K, 600 K, and 800 K) and at strain levels varying between -10% and 10%. The analysis of interface TBR contradicts the usual notion that each interface contributes equally to the heat transfer resistance in a layered structure. The comparison of thermal behavior of superlattices and nanocomposites indicate that the morphology differences lead to a striking contrast in the phonon spectral density, interfacial thermal boundary resistance, and thermal conductivity. Both compressive and tensile strains are observed to be important factors in tailoring the thermal conductivity of the analyzed superlattices, whereas have very insignificant influence on the thermal conductivity of the analyzed nanocomposites.

Three-Dimensional Materials Science VI: Novel Tools for 3D Data Acquisition and Analysis - Part I

Sponsored by: The Minerals, Metals and Materials Society, ASM International, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, ASM-MSCTS: Texture and Anisotropy Committee, TMS/ASM: Phase Transformations Committee
Program Organizers: Alexis Lewis, Naval Research Laboratory; Anthony Rollett, Carnegie Mellon University; David Rowenhorst, Naval Research Lab; Jeff Simmons, AFRL; Stuart Wright, EDAX Inc-TSL

Wednesday AM	Room: 401
February 17, 2010	Location: Washington State Convention Center

Session Chairs: Alexis Lewis, U S Naval Research Laboratory; John Budai, Oak Ridge National Laboratory

8:30 AM Invited
3-D Materials Science using Polychromatic Synchrotron X-Ray Microdiffraction: *John Budai*[1]; Jon Tischler[1]; Wenjun Liu[2]; Anthony Rollett[3]; [1]Oak Ridge National Laboratory; [2]Argonne National Lab; [3]Carnegie Mellon University

Synchrotron x-ray microdiffraction facilities continue to make progress in providing new techniques for quantitative, 3-D structural studies in materials science. In particular, we have developed a polychromatic, scanning microdiffraction and microfluorescence beamline with submicron spatial resolution at the Advanced Photon Source. X-ray area detectors such as the one recently implemented on our beamline are capable of collecting raw images at rates exceeding 5 GB/min. Such large datasets require rapid, automated analysis techniques in order to obtain 3-D spatially-resolved lattice, orientation, and strain maps. This presentation will review progress in 3-D Laue micro- and nano-diffraction techniques and will illustrate how nondestructive x-ray microscopy can provide unique measurements in the areas of thermal grain growth and phase separation. The goal of these studies is to provide experimental datasets for comparison with computational theory and modeling.Support at ORNL, UT-Battelle by DOE-BES, Materials Sciences and Engineering Division; UNI-XOR support at APS by DOE-BES.

9:00 AM
Applications of a Local-Electrode Atom-Probe (LEAP) 4000X Si for Obtaining Three-Dimensional Chemical Information with Subnanoscale Resolution: *David Seidman*[1]; [1]Northwestern University

Results obtained utilizing the first commercial LEAP 4000X Si, installed in the Northwestern University Center for Atom-Probe Tomography in early July 2009, are presented. This instrument utilizes a short wavelength picosecond solid-state laser to dissect specimens on an atomic scale, one atom at a time, at pulse repetition rates of up to 1000 kHz. The LEAP 4000X Si has many unique advantages over earlier versions of LEAP tomographs. Particularly, it has a smaller spot size, significantly improved mass resolution (1/1800 FWHM for Al), and a larger signal-to-noise (S/N) ratio. The smaller spot size produces more localized laser-beam heating, which results in a lower background and improved mass resolution. The larger value of the S/N ratio implies a smaller minimum detectable mass. The 4000X Si is used for analyzing high-strength low-carbon steels, nickel-based and aluminum-scandium-based alloys, silicidation reactions, low-energy implants in silicon, and magnesium oxide layers in magnetic tunnel junctions.

9:20 AM
Partitioning Behavior of Al and Si in FINEMET Nanocrystalline Soft Magnetic Alloys, as Studied by Atom-Probe Tomography: *Keith Knipling*[1]; Maria Daniil[1]; Matthew Willard[1]; [1]Naval Research Laboratory

FINEMET is a nanocrystalline soft magnetic material comprised of ~70 vol.% randomly oriented $D0_3$ Fe-Si grains (~10 nm) embedded in a residual B- and Nb-rich amorphous matrix. Owing to the small grain size, the magnetocrystalline anisotropy is averaged out by exchange interactions and the alloys possess a unique combination of large magnetization, high permeability, and low core losses. Substituting Al for Fe further decreases the magnetocrystalline anisotropy of the nanocrystals. We employ three-dimensional atom-probe tomography to quantify the phase compositions obtained in a series of $(Fe,Si,Al)_{87}B_9Nb_3Cu_1$ alloys. Relationships between the compositions of the nanocrystals and the observed bulk magnetic properties (saturation magnetization and coercivity) are discussed. The wide field-of-view of modern atom-probes now also enables detailed structural analysis, including measurement of grain size, volume fraction, number density, and edge-to-edge intergranular distances directly in three dimensions. We correlate these measurements to structural information obtained by X-ray diffraction and transmission electron microscopy.

9:40 AM
Recent Advances in Atom Probe Tomography for 3D Microstructural Characterization: *Michael Miller*[1]; [1]ORNL

Atom probe tomography is one of the most direct methods for the characterization of fine scale microstructures, as the technique generates the atomic coordinates and mass-to-charge state and hence the elemental identity of the atoms in the sampled volumes. Recent advances in atom probe instrumentation enable datasets into the billion atom range to be collected. Several statistical methods have been developed to extract important microstructural information of the features present in these data. These data can be directly compared to atomistic models and simulations of the microstructure. A review of the recent major advances in local electrode atom probe (LEAP®) instrumentation and data analysis techniques and the resulting improvements in performance will be presented.Research at the Oak Ridge National Laboratory SHaRE User Facility was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

10:00 AM
Atom Probe Studies on the Segregation of C and N in Fe-17%Mn Steels: *Jae-Bok Seol*[1]; Soon-Ki Lee[2]; Chan-gyung Park[3]; [1]POSTECH; [2]POSCO; [3]POSTECH, NCNT

It has been widely known that Fe-17wt.%Mn steels exhibit a good damping capacity, which is caused by the movement of γ/ε interface formed on cooling. Since undesired C and N are often added to the steels during commercial fabrication process, the damping capacity of the steels is deteriorated. However, the effects of C and N on the damping sources have not been understood yet. In the present study, atom probe tomography with tunable laser, high spatial resolution of 2~3 nm, was applied to investigate the exact position and quantitative information of impurity atoms in Fe-17%Mn. The current results have demonstrated that APT techniques have made it possible to identify and quantify the exact state of C and N with three dimensional tomography imaging and composition profile in the atomic scale. The discussion on segregation of C and N at the γ/ε interface and e martensite phase will be followed.

10:20 AM Break

10:50 AM
Correlative Microscopy: 3-D Multiscale Imaging and Modelling: *Farid Tariq*[1]; Ralph Haswell[2]; Peter Lee[1]; David McComb[1]; [1]Imperial College London; [2]Shell Global Solutions International B.V.

Materials are often inadequately described using 2-D imaging and furthermore their properties can depend on their structure on multiple length scales. In this study several tomographic techniques will be combined to investigate 3-D structure on length scales that span four orders of magnitude. Heterogeneous ceramic catalysts are an ideal system to analyse as they represent a material where functionality is dependant on multiscale flow of molecules through a hierarchical pore structure. Consequently, multiscale characterisation of their structure can provide key insights for future catalyst design. Ceramic catalysts were analysed using (i) synchrotron x-ray microtomography (XMT); (ii) serial sectioning using dual beam focused ion beam (DB-FIB); and electron tomography (ET). Each respective technique provides information at different scale lengths for different volume sizes. Shapes, structures and morphology can be characterised and the structure modelled to provide useful insights into catalyst performance and lifetime.

11:10 AM
Multi-Scale Characterization of a Ni-Base Single Crystal Turbine Blade: *Michael Groeber*[1]; Dennis Dimiduk[1]; Chris Woodward[1]; Michael Uchic[1]; Rebecca Fahringer[1]; [1]AFRL

Multi-scale modeling of materials dictates the need for multi-scale characterization of structure. Over the past decade, multiple tools for collecting 3D structure information at various scales) have matured, but without a concerted effort to link their resultant data. This work will focus on the collection of 3D structure information across multiple scales and the integration of the data into a systems level representation of the material. Specifically, this talk will focus on the experimental collection of the 3D structure information for a Ni-base superalloy turbine blade. The characterization process employed in this study is truly multi-scale in nature and requires the integration of various investigatory techniques. The microstructural features of interest span 3-4 orders of magnitude and are visible after different preparation steps and under different imaging conditions. This presentation will outline the approach necessary to characterize this material at the systems level in a robust fashion.

11:30 AM
Multi-Length Scale Three Dimensional Characterization of Tantalum Carbide Microstructures: *Robert Morris*[1]; Gregory Thompson[1]; [1]The University of Alabama

Tantalum carbide compounds have been fabricated by either hot-isostatic pressing (HIP), spark plasma sintering (SPS), and vacuum plasma spraying (VPS) of constituent powders. Depending upon the targeted stoichiometry (TaC or Ta2C or mixed) and fabrication process, a single or dual phase microstructure can be formed. The duplex microstructure was found to be either acicular grains in HIP processes or laths within equiaxed grains for arc based processing. The microstructures have been analyzed across different length scales. Atom probe tomography has revealed preferential segregation of powder impurities, including iron, to the grain boundaries. STEM-HAADF tomography has revealed that the laths are tens of nm thick and can terminate through mutual intersections. Serial sectioning FIB based techniques reveal the global structure in which the laths do not necessarily span the entire grain. The collective combination of 3D techniques will describe the formation and stability of tantalum carbide microstructures.

11:50 AM
A Crystal-Plasticity FEM Study on Effects of Simplified Grain Representation and Mesh Types on Mesoscopic Deformation Heterogeneities: *Yoon Suk Choi*[1]; Michael Groeber[2]; Dennis Dimiduk[2]; Christopher Woodward[2]; Michael Uchic[2]; Triplicane Parthasarathy[1]; [1]UES, Inc.; [2]Air Force Research Laboratory

Polycrystalline microstructure-based elastic or elasto-viscoplastic FEM approaches have been a subject of numerous studies since these approaches provide crucial information regarding the development of mesoscopic deformation heterogeneities and its microstructural dependence. However, only few preliminary parametric studies have attempted to clarify and understand numerical artifacts, which might be caused by simplified grain geometries, intractable meshes and ad-hoc RVE selection. The present study systematically investigated the influence of the simplification of grain boundary morphologies and the selection of different mesh types on the distribution of simulated flow heterogeneity across the grain boundary. A bicrystal sphere embedded in a cubic box was utilized to perform the current preliminary parametric study. Simulation results were analyzed using various statistical characterization techniques.

Ultrafine Grained Materials – Sixth International Symposium: Young Scientist

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee, TMS: Nanomechanical Materials Behavior Committee, TMS: Shaping and Forming Committee
Program Organizers: Suveen Mathaudhu, U.S. Army Research Laboratory; Mathias Goeken, University Erlangen--Nürnberg; Terence Langdon, University of Southern California; Terry Lowe, Manhattan Scientifics, Inc.; S. Semiatin, Air Force Research Laboratory; Nobuhiro Tsuji, Kyoto University; Yonghao Zhao, University of California - Davis; Yuntian Zhu, North Carolina State University

Wednesday AM — Room: 606
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Terry Langdon, University of Southern Californis; Suveen Mathaudhu, U.S. Army Research Laboratory; Yuntian Zhu, North Carolina State University; Terry Lowe, Manhatten Scientifics, Inc.

8:30 AM
Grain Growth Kinetics for an Aluminum Based Nanocmposite: *Leyla Hashemi-Sadraei*[1]; Rustin Vogt[1]; Zhihui Zhang[1]; Ying Li[1]; S. Ebrahim Mousavi[1]; Enrique Lavernia[1]; Julie Schoenung[1]; [1]University of California, Davis

An aluminum based nanocomposite has been produced by cryomilling powders of aluminum 5083 and boron carbide. This material when consolidated is known to exhibit super-high strength and good stiffness due to the ultrafine grained (UFG) structure of aluminum and incorporation of B4C reinforcement, respectively. The thermal stability which is essential for UFG materials has been studied for these nanocomposite powders by annealing at various temperatures for select times. The effect of cryomill-generated second phase particles on thermal stability of UFG aluminum grains was investigated. Further, grain growth kinetics and mechanisms were studied based on the experimental results and existing grain growth equations. For this purpose, grain size values were calculated and compared using several X-ray-based methods in addition to observation with transmission electron microscopy. The results provided a better understanding of grain size calculation techniques and confirmed the expected high thermal stability of this material.(I'd like to be considered for the Young Scientist Session)

8:45 AM
Influence of High-Pressure Torsion on Hardness of a Supersaturated Al-7136 Alloy: *Zhi Duan*[1]; Xiaozhou Liao[2]; Megumi Kawasaki[1]; Roberto Figueiredo[1]; Terence Langdon[1]; [1]University of Southern California; [2]University of Sydney

The potential for further strengthening of the 7000 series Al alloys using severe plastic deformation makes it attractive to apply high-pressure torsion

(HPT) to the Al-7136 alloy. In addition to HPT processing, different pre-processing was conducted by equal-channel angular pressing including 1 pass at room temperature and 4 passes at 473 K. Hardness contour mapping was used to demonstrate the presence of a complicated microhardness evolution which depended upon the pre-processing as well as the strains imposed in processing. The effect of HPT on the Al-7136 alloy is discussed based on TEM images of the grains and precipitates. It is shown that HPT processing significantly refines the grain size to a minimum size of less than 40 nm in some parts of the sample and promotes grain boundary segregation of excessive alloying elements.

9:00 AM
Microstructural Characterization of Ti-6Al-4V Metal Chips by Focused Ion Beam and Transmission Electron Microscopy: *Lei Dong*[1]; Judy Schneider[1]; Jane Howe[2]; [1]Mississippi State University; [2]Oak Ridge National Laboratory

It has been reported that chips formed during metal cutting contain nanocrystalline structures. This current study utilizes focused ion beam (FIB) techniques to prepare transmission electron microscopy (TEM) thin foils from various regions and orientations of cut Ti-6Al-4V metal chips to verify the crystalline nature of the chips. Images of the resulting microstructure were obtained via TEM and used to construct a 3-dimensional image. A range of grain sizes and morphologies were observed, which are consistent with an inhomogeneous deformation process. A comparison of the results obtained at different length scales will be presented. Research supported in part by ORNL's SHaRE User Facility, which is sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, the U.S. Department of Energy.

9:15 AM
UFG Aluminum Alloy Tested in Dynamic High Temperature Compression: *Emily Huskins*[1]; K. Ramesh[1]; [1]Johns Hopkins University

Materials with ultra-fine grained (UFG) nanostructures have been of interest for many years due to their improved strengthening over their coarse-grained counterparts. However, these UFG materials also exhibit different strain rate sensitivity and deformation mechanisms, both of which affect the stability of plastic deformation and therefore ultimate failure of the material. Such plastic instabilities may be localized and experience a significant temperature rise due to plastic work during nearly-adiabatic dynamic deformations. However, there are limited studies of the material response of UFG materials at both high temperatures and high strain rates. In this work an UFG aluminum alloy is tested under dynamic compression ($10^3 s^{-1}$) loading at elevated temperatures (298K – 673K). The material response including strain rate sensitivity and thermal softening are discussed.

9:30 AM
Work-Hardening Stages of AA1070 and AA6060 after Severe Plastic Deformation: *Matthias Hockauf*[1]; Lothar W. Meyer[1]; Ines Schneider[2]; [1]Chemnitz University of Technology; [2]Wehrwissenschaftliches Institut für Werk- und Betriebsstoffe

Based on the concept of work-hardening for f.c.c. metals the commercially pure aluminium AA1070 (soft annealed) and the aluminium alloy AA6060 (peak aged) were investigated. Equal-Channel Angular Pressing (ECAP) was used to introduce very high strains and an ultrafine-grained microstructure. Subsequently compression tests were performed in a wide range of strain rates between 10-4 and 103 s-1. The results indicate that strain path and the corresponding dislocation structure is important for the post-ECAP yielding and the following hardening response. Furthermore the precipitates of the AA6060 clearly constrain the interactions of dislocations in work-hardening stage III – causing lower strain rate sensitivity. If compared to the AA1070 they avoid hardening in stage V where an additional rate and temperature depending effect contributes – caused by the interaction of deformation induced vacancies and dislocations.

9:45 AM
Unusual Macro-Structure and Hardness Patterns in Duplex Stainless Steel Processed by High-Pressure Torsion: *Yang Cao*[1]; Yanbo Wang[1]; Saleh Alhajeri[2]; Xiaozhou Liao[1]; Simon Ringer[1]; Terence Langdon[3]; Yuntian Zhu[4]; [1]The University of Sydney; [2]University of Southampton; [3]University of Southern California; [4]North Carolina State University

We report a surprising observation that double swirl shear strain patterns and local shear vortices form in duplex stainless steel disks processed by high-pressure torsion (HPT). This contradicts our conventional belief that the processing strain only varies with the distance form the disc center. Duplex stainless steel disks with appropriately the same volume fraction of austenite and ferrite phases were processed using HPT for a series of from 2 to 20 revolutions. The macroscopic shear strain induced by HPT and its evolution were visualized using optical microscopy. Microstructural evolution was characterized using transmission electron microscopy (TEM). Hardness evolution of the two phases was investigated using nanoindentation and the results were correlated with the local structural features observed from TEM.

10:00 AM
Improvement of Strength and Ductility for an AA6065 Aluminium Alloy Achieved by a Combination of Equal-Channel Angular Pressing and Ageing Treatment: Lothar W. Meyer[1]; *Kristin Hockauf*[1]; Matthias Hockauf[1]; Thorsten Halle[1]; [1]Chemnitz University of Technology

Incited by the aim of improving the strength and preserving a moderate ductility, the promising approach of a combined ECAP (equal-channel angular pressing) and ageing treatment was applied to AA6056, an AlMgSi(Cu)-alloy. In this presentation, the evolution of hardness during post ECAP ageing and the effect of ageing temperature and time on strength and ductility will be discussed. By means of scanning transmission electron microscopy, the underlying microstructural features in terms of grain size and precipitation characteristics of coherent β'' and semicoherent Q' precipitates will be presented. It was found that peak-ageing especially at low ageing temperatures is suitable for achieving the desired high-strength combination, whereas – on the expense of some percent in the strengthening- the ductility is best in slightly underaged conditions. Compared to the initial peak-aged condition, an increase in strength of 30%, combined with a moderate ductility of 7% uniform elongation could be achieved.

10:15 AM Break

10:30 AM
Aging of an Al-Si-Mg Alloy Processed by ECAP: The Effect of the Initial Microstructure: *Edgar Garcia-Sanchez*[1]; Edgar Ortiz-Cuellar[1]; Edgar Lopez-Chipres[2]; Martha P. Guerrero-Mata[1]; Rafael Colás[1]; [1]FIME-UANL; [2]Facultad de Quimica, Univerisdad Juarez del Edo. deDurango

With the aim to study the second phase particles effect on the grain refinement and mechanical properties in Aluminum alloy, in this work a commercial Al-Mg-Si alloy under various initial microstructural conditions has been deformed at room temperature by multi-pass 90º equal channel angular pressing (ECAP). The alloy after ECAP was aging under different conditions. The post ECAP annealing heat treatments in some cases promote high strengths and relatively high ductility; these were evaluated by means of tensile tests carried out at room temperature. The grain refinement was promoted by the presence of particles as observed by SEM and TEM. With this work was possible to obtain the optimal conditions for processing an Aluminum alloy under SPD and post aging heat treatments improving the mechanical properties.

10:45 AM
Grain Size Effect on the Deformation Mechanisms and Mechanical Properties of Gum Metals: *Yanbo Wang*[1]; Xiaozhou Liao[1]; Yonghao Zhao[2]; Enrique Lavernia[2]; Ruslan Valiev[3]; [1]The University of Sydney; [2]University of California, Davis,; [3]Ufa State Aviation Technical University

Gum Metals are an emerging class of multifunctional titanium alloys with superior mechanical properties including super elasticity, super strength, and superplastic-like cold workability, which arise from their unusual deformation mechanisms. It has been well-established that reducing grain sizes down to the ultrafine-grained (< 1 µm) and nanocrystalline (< 100 nm) regimes affects significantly the deformation mechanisms of materials, and that this in turn affects mechanical properties of the materials. In this presentation, we will report our investigation results on the effect of grain size reduction on the deformation mechanisms and mechanical properties of Gum Metals. Grain size reduction is achieved via severe plastic deformation. Deformation mechanisms and mechanical properties are investigated using in-situ and ex-situ transmission electron microscopy and hardness test.

11:00 AM
Equal Channel Angular Pressing of Pure Gold: *Anumalasetty Nagasekhar*[1]; T. Rajkumar[2]; D. Stephan[2]; Y. Tick-Hon[3]; [1]The University of Queensland; [2]Heraeus Materials Singapore Pte Ltd; [3]University of Toronto

Equal channel angular pressing (ECAP) is the most promising severe plastic deformation (SPD) technique for fabrication of bulk ultrafine and nanostructured materials, compaction of powders, and mechanical property enhancement of tubular materials. Large variety of materials has been processed through ECAP to fabricate ultrafine and nano structures. In current studies, the precious metal pure gold (99.99% purity) is processed upto twelve ECAP passes via Route Bc (90 degree clock wise rotation between successive passes). The microstructural and mechanical properties changes in the pure gold with increase in ECAP passes have been reported.

11:15 AM
Synthesis of Bulk Nanostructured Cu via Spark Plasma Sintering and High Pressure Torsion of Cryomilled Powders: *Haiming Wen*[1]; Yonghao Zhao[1]; Osman Ertorer[1]; Troy Topping[1]; Ruslan Valiev[2]; Enrique Lavernia[1]; [1]University of California at Davis; [2]Ufa State Aviation Technical University

Bulk nanostructured materials can be prepared using a variety of severe plastic deformation methods. These can be grouped into two general categories, discrete powder methods (e.g., cryomilling and cold finger deposition) and solid state transformation methods (e.g., equi-channel pressing). Powder consolidation methods provide benefits, such as control of grain size distribution, resistance against grain growth and scale-up potential; however, some disadvantages include contamination and incomplete particle bonding which can lead to porosity. In this study, we use spark plasma sintering (SPS) and high pressure torsion to synthesize bulk dense nanostructured Cu. The Cu powders, with an average grain size of 20 nm, were prepared via cryomilling in liquid nitrogen. High-pressure SPS is used to prepare bulk NS Cu. In addition, high pressure torsion was used to consolidate dense NS Cu at its super-plasticity regime. Mechanical properties and microstructures are measured and compared with particular emphasis on operative deformation mechanisms.(I'd like to be considered for the Young Scientist Session)

11:30 AM
Continuous High Pressure Torsion: *Kaveh Edalati*[1]; Zenji Horita[1]; [1]Kyushu University

Continuous high pressure torsion (CHPT) was developed as a severe plastic deformation process (SPD) so that the ribbons of high purity Al, Cu and Fe with rectangular cross sections, 0.6mm thickness and 3mm width, were successfully processed by introducing intense strain under high pressure. It is shown that the results of hardness measurements by CHPT are well consistent with those of conventional HPT using disc and ring specimens. Microstructural observations using transmission electron microscopy demonstrate that CHPT can be used as a continuous SPD process for grain refinement.

11:45 AM
Unconventional ECAE Processing of Magnesium Alloys: *David Foley*[1]; Majid Al-Maharbi[1]; K.T. Hartwig[1]; Ibrahim Karaman[1]; Hans Maier[2]; L.J. Kecskes[3]; Suveen Mathaudhu[3]; [1]Texas A&M University; [2]University of GH Paderborn; [3]US Army Research Lab

While SPD matured as a research area, standard deformation techniques were adopted by groups worldwide. In ECAE/ECAP this includes die angles, processing routes, and workpiece geometries. Although this standardization allows for intra-lab repeatability and understanding, it can influence a researcher's thought process: "What route/temperature is best?" rather than "What microstructure and texture am I seeking and what deformation modes and strain paths do I need to get there?" The researcher's approach becomes especially important in materials with limited slip systems, high mechanical anisotropy, or variable room-temperature phase concentration and morphology. An examination of conventional and unconventional ECAE processing in magnesium alloys will illustrate the importance of customized processing methods for achieving desired textures and microstructures. Hybrid routes, intra-pass temperature variation, and SPD + Rolling allow for greater control over the material's resulting mechanical properties.

12:00 PM
Thermal Stability of Ultrafine Grained 316 Austenitic Stainless Steel: *Auriane Etienne*[1]; Bertrand Radiguet[1]; Ruslan Valiev[2]; Cécile Genevois[1]; Jean-Marie Le Breton[1]; Philippe Pareige[1]; [1]GPM UMR CNRS 6634; [2]Institute of Physics of Advanced Materials

Austenitic Stainless steels (ASS) in internal structures of pressurized water reactor are susceptible to irradiation-assisted stress corrosion cracking (IASCC). Even if this complex form of material degradation is still not well understood, only the combination of all irradiation-induced microstructural changes (point defect (PD) and solute clustering, segregation at grain boundaries (GB)…) can lead to IASCC. Since all these changes are essentially due to PD super-saturation, increasing PD annihilation at GB could limit IASCC. A 316 ASS has been nano-structured by high pressure torsion and ion irradiated at 350°C. The evolution of the grain size under the ion irradiation has been measured. However, this evolution may be the result of a combination of thermal and irradiation effects. Thus, the thermal stability of this nano-material was investigated using complementary techniques (transmission electron microscopy, X-ray diffraction and Mössbauer Spectroscopy). Results after thermal ageing between 350 up to 900°C will be presented and discussed.

12:15 PM
A Study of the Thermal Stability of Nano-Twinned Copper: *Christopher Saldana*[1]; Sergey Suslov[1]; Matthew Hudspeth[1]; Eric Stach[1]; Srinivasan Chandrasekar[1]; [1]Purdue University

Inadequate thermal stability has precluded the widespread application of nanostructured materials. The use of conventional stabilization methods has generally only been feasible in multi–component nanostructured systems, leaving single-component systems without an effective route to thermal stabilization. In this study, stabilization in high purity copper is demonstrated through the stability afforded by a dense network of twin boundaries. A range of microstructures, including one dominated by twins, is produced in the copper by carrying out deformation under a wide set of conditions – strain rates varying from 10 to 10^3 per second, strains from 1 to 7 and temperatures as low as cryogenic. Stability of these microstructures is evaluated by microstructure observation, strength measurement and calorimetry. Changes in microstructure and hardness stability, as well as a switchover from grain boundary mediated diffusion to twin diffusion, is demonstrated in the case of heavily twinned copper.

2010 Functional and Structural Nanomaterials: Fabrication, Properties, Applications and Implications: Characterization of Nanomaterials

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Nanomaterials Committee
Program Organizers: David Stollberg, Georgia Tech Research Institute; Nitin Chopra, University of Alabama; Jiyoung Kim, University of Texas - Dallas; Seong Jin Koh, University of Texas at Arlington; Navin Manjooran, Siemens Corporation; Ben Poquette, Keystone Materials; Jud Ready, Georgia Tech

Wednesday PM — Room: 214
February 17, 2010 — Location: Washington State Convention Center

Session Chair: Nitin Chopra, University of Alabama; Jiyoung Kim, University of Texas - Dallas

2:00 PM Introductory Comments

2:05 PM
The Investigation on Internal Structure of Spherical Graphites in Ductile Cast Iron by Transmission Electron Microscopy: *Ali-Reza Kaini-Rashid*[1]; Arash Elhami-Khorasani[1]; [1]Ferdowsi University of Mashhad

Microstructure of cast irons often consists of two totally different phases: Metallic matrix (like steel microstructures), and graphite with semi metallic properties. In the process of preparing the specimens for observing by TEM, maintenance of graphite particles before reaching adequate thinness is not quiet easy. In the present study, by choosing the specific techniques, it has been attempted to maintain the spherical graphites in their primer locations, while reaching extreme thinness. This leads to the ability of having a clear microscopic observation of the graphites' internal structure, especially on the outer layers. Further studies reveal these graphites; consist of a laminar internal structure with a special rotation pattern along crystal planes.

2:25 PM
Selective Placement of Single Nanoparticles of Different Sizes: *Pradeep Bhadrachalam*[1]; Seong Jin Koh[1]; [1]University of Texas at Arlington

For practical applications involving nanoscale building blocks such as nanoparticles, nanotubes, and nanowires, it is necessary to place these building blocks onto desired substrate locations. We demonstrate a new technique for precise placement of individual nanoparticles of different sizes onto different target locations on the same substrate. This was done in a self-limiting manner using wet chemistry and CMOS-compatible parallel processing. Au nanoparticles (AuNPs) with ≈20nm and ≈50nm in diameter were used as a model system. This size-selective placement was achieved using electrostatic guiding structures which first guide single ≈50nm AuNPs onto targeted locations and then single ≈20nm AuNPs onto different target locations. Theoretical analysis revealed that the change in the free energy barrier after the placement of a single nanoparticle onto a targeted location is responsible for self-limiting size-selective placement of nanoparticles.

2:45 PM
Activation Energy for Crystallization in Nanocrystalline Exchange Coupled Magnets: *Matthew Willard*[1]; Maria Daniil[2]; B. Hornbuckle[3]; Juan Saavedra[4]; [1]Naval Research Laboratory; [2]George Washington University; [3]University of Alabama - Tuscaloosa; [4]University of Puerto Rico - Mayaguez

Nanocrystalline soft magnetic alloys have been studied for their excellent magnetic performance. Amorphous materials are processed using the rapid solidification technique melt spinning. The rapidly solidified alloys are isothermally annealed to improve their magnetic performance by partially devitrifying the ribbon samples. To examine the crystallization kinetics, constant heating rate experiments were performed with heating rates varied between 2 and 85°C/min from 50 to 900°C. In this study, the crystallization kinetics of alloys with composition (Fe, Co, Ni)-Zr-B-(Cu) are determined by Kissinger analysis. The thermally activated primary crystallization temperature was observed for each sample at numerous heating rates to provide accurate activation energies. Fe-rich alloys have activation energies (3.0-3.5 eV/atom), while Ni-rich alloys have lower activation energies (2.1-2.5 eV/atom). The reduced activation energy likely results from the more active diffusion in Ni-based alloys and may be a reason for the deteriorated nanocrystalline alloy formation at these compositions.

3:05 PM
Tunneling Spectroscopy of Colloidal Nanoparticles: *Ramkumar Subramanian*[1]; Pradeep Bhadrachalam[1]; Seong Jin Koh[1]; [1]The University of Texas at Arlington

For practical applications of nanoparticles such as in nanoelectronics, photonics, and bio-medicine, knowledge of their electronic structure plays a critical role. We demonstrate a new solid-state tunneling spectroscopic technique for individual nanoparticles that not only enables direct probing of the energy levels of a single nanoparticle, but many such measurement units can be fabricated in a single-batch process. Resonant tunneling between the vertically separated electrodes and the nanoparticle placed between these electrodes forms the basis of spectroscopic measurements. Spectroscopic units with ≈ 7 nm CdSe nanoparticles were used as a model system. Current-voltage measurements for these units yielded the energy level spacings and the band gap by numerical differentiation of the I-V plots. These will be compared with measurements using the lock-in method that directly measures differential conductance.

3:25 PM
Grains Size Effect on Density of Geometrically Necessary Dislocations: *Eduard Kozlov*[1]; Nina Koneva[1]; [1]Tomsk State University of Architecture and Building

The scalar density of dislocations can be divided on two components: statistically stored dislocations (SSD) also geometrically necessary dislocations (GND). SSD are braked by rather weak barriers - other dislocations. If at metal or an alloy there are stronger barriers there is accumulation of GND. Density GND is proportional to a deformation gradient. The density of excess dislocations is proportional to curvature-torsion of a crystal lattice or a deformation gradient. In work methods of measurement of density as GND, and excess dislocations are considered. Measurements of these sizes on polycrystals of pure metals, solid solutions and steels are spent. Dependence of GND density on the grain size the size of dislocation fragments and dislocations cells is established. It is shown, that fraction of GND increases when sizes of structural element crushes. At that the general density of dislocations decreases and the density of partial disclinations especially joint disclinations increases.

3:45 PM Break

4:00 PM
A Comparative Study of Characterization of CNT Turfs by Means of SEM Analysis and Stereological Techniques: *H. Malik*[1]; K. Stephenson[1]; D.F. Bahr[1]; D.P. Field[1]; [1]Washington State University

The numerous novel and emerging properties of carbon naotubes have placed this relatively new breed of technological materials under great focus. For applications in the regime of micro-electro-mechanical systems (MEMS) including electrical and thermal contact switches, and sensors, it is crucial to understand the combined collective behavior of CNT turfs rather than the mechanical properties of a single tube. In this present study, we have investigated the existing correlation between the mechanical behavior of multi-walled carbon nanotube (MWCNT) turfs and stereological parameters. Image analysis techniques using SEM were employed in connection with 2D planar and projected images. Also, stereological measures were incorporated to collect information from projected sections of images. These measures serve as a comprehensive source of information regarding turf density, tortuosity, connectivity, i.e. interaction between individual CNT segments, complexicity, nanotopology, etc.

4:20 PM
Nucleation Energetics and Kinetics of Solidification in Nanoscale Metallic Droplets: *Ritesh Sachan*[1]; J. Strader[1]; H. Krishna[2]; A.K. Gangopadhyay[2]; R. Kalyanaraman[1]; [1]University of Tennessee-Knoxville; [2]Washington University

Over the past century, solidification process has been qualitatively investigated by classical nucleation theory . In the present work we discuss nucleation energetics and kinetics by a modified CNT for the solidification of nanoscale elemental metallic droplets of Ag, Co and Ni on as SiOsurface. Such nanostructures have important applications in the field of plasmonics, magnetic data storage and catalysis. This theory includes the effect of the density change during solidification and liquid droplet size. Our theory shows strong size-dependent nucleation energetics and kinetics, and that the interface between liquid and vacuum is the most favorable nucleation site. Experimental measurements, of number and size of grains forming within solidified hemispherical metallic droplets, were made for drops prepared by nanosecond pulsed laser-induced melting and self-organization. The experimental results also show strong size-dependence of nucleation rate consistent with our modified CNT theory.

4:40 PM
Preparation, Characterization and Antibacterial Properties of Ag-Doped MgO/TiO2 Nanoparticles: Guoliang Li[1]; *Peng Bing*[1]; Liyuan Chai[1]; Yajun Gu[1]; [1]Central South University

Ag-doped MgO/TiO2 nanoparticles were successfully prepared via hydrothermal precipitation using titanium sulfate, magnesium chloride and silver nitrate as raw materials. The effects of various conditions on the preparation process of the Ag-doped MgO/TiO2 nanoparticles are investigated. The results showed that the optimal conditions were as follows: pH 9.0, mass ratio of titanium to silver 0.02, mass ratio of titanium to magnesium 2:1, reaction temperature 80°, mass ratio of surfactant to titanium and magnesium 3%, calcination temperature 500°. The as-obtained Ag-doped MgO/TiO2 nanocomposites were well characterized by X-ray diffraction, scanning electron microscopy and energy dispersive X-ray. The antibacterial experiments exhibit that the composite has a higher antibacterial activity than that of both the Ag-doped TiO2 nanoparticles and the mechanical mixture of Ag-doped TiO2 and MgO.

5:00 PM
Synthesis and Performance Study of Sn-Doped Nanometer Rutile TiO2 Powder: *Wu Daoxin*[1]; [1]Changsha University of Science and Technology

In this paper, originated from Ti(Bu)4, nano-rutile Sn-TiO_2 was synthesized by low temperature hydrolytic process. Then they were characterized by means of X-ray diffratction, UV-vis diffuse reflectance, fluorescence spectrum. Results showed that with the increase of the doped concentration of Sn, the reflectance of DRS decreased accordingly, while the powder's increase in light absorbance. Absorption of light broad to the visible region, which indicated that red shift occurred. The fluorescence spectrum intensity of Sn-TiO_2 increased according to the doped concentration. Sn-TiO_2 change the crystalline form when Calcined at different temperatures: in the low temperature for anatase; as the temperature rising, it transist to rutile, while at 800°, it is almost entirely rutile. With the increase of the calcination temperature, the Absorption of DRS increased, while the fluorescence spectrum intensity of $Sn-TiO_2$ decreased accordingly.

5:20 PM Concluding Comments

Advanced Materials and Fuels Enabling Future Fusion, Fission and Hybrid Reactor Systems: Diagnostics and Structural Materials

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS/ASM: Computational Materials Science and Engineering Committee, TMS/ASM: Corrosion and Environmental Effects Committee, TMS: High Temperature Alloys Committee, TMS/ASM: Nuclear Materials Committee

Program Organizers: Joseph Farmer, Lawrence Livermore National Laboratory; Thomas M. Anklam, Lawrence Livermore National Laboratory; Magdalena Serrano de Caro, Lawrence Livermore National Laboratory

Wednesday PM — Room: 3A
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Joseph Farmer, Lawrence Livermore National Laboratory; Magdalena Serrano de Caro, Lawrence Livermore National Laboratory

2:00 PM Introductory Comments

2:05 PM Plenary

MaRIE (Matter-Radiation Interactions in Extremes): An Experimental Facility Concept: *Jack Shlachter*[1]; [1]Los Alamos National Laboratory

MaRIE, for matter-radiation interactions in extremes, is Los Alamos National Laboratory's concept for an experimental facility complex which will provide transformational materials solutions to address national security, energy security, and discovery science needs in the coming decades. The historical approach to developing materials with required lifetime and performance characteristics relied heavily on observation and subsequent validation of empirical models. This approach will not be sufficiently timely or cost effective to solve future problems in fusion, fission, or hybrid reactor systems, and it is widely recognized that predictive tools and material fabrication control will be required. MaRIE is being designed to bridge the "micron" gap between atomistic calculations and continuum models, thereby facilitating this paradigm shift. The three components of the facility complex as currently envisioned will be described and include a state-of-the-art synthesis and characterization capability, a multi-probe hall which can subject samples to dynamic shock conditions, and a spallation irradiation environment with in situ diagnostic capability, the latter dedicated to providing access to a radiation region of relevance to fission, fusion, and hybrid systems. The entire MaRIE complex is predicated on a predictive theory, modeling and simulation capability.

2:45 PM Invited

TEM Study of Oxide Nanoparticles in ODS Steels Developed for Radiation Tolerance: *Luke Hsiung*[1]; Michael Fluss[1]; Joshua Kuntz[1]; Bassem El-Dasher[1]; William Choi[1]; Scott Tumey[1]; [1]Lawrence Livermore National Laboratory

Many issues remain unsolved for developing ODS steels for fission and fusion applications including the role of fusion relevant helium and hydrogen gases on the deformation and fracture of irradiated material and mechanisms of swelling suppression in ODS steels. To resolve these issues, we plan to investigate microstructural changes of ODS steels driven by ion-beam irradiation. In preparation for the experiments, we are performing high resolution electron microscopy to study ODS steels with an emphasis on oxide/matrix interfacial structure. We will point out the features which may influence the growth and refinement of nano-particles. We will also point to those features that are of interest with respect to the suppression of radiation-induced swelling due to the nano-particles according to the new results obtained from the He+Fe irradiation experiments. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DEAC5207NA27344.

3:15 PM Invited

A Small Angle X-Ray Scattering Study of Helium/Nano-Oxide Structure in ODS Steels: *B. S. El-Dasher*[1]; J. D. Kuntz[1]; M. Caro[1]; S. O. Kucheyev[1]; T. Van Buuren[1]; T. M. Willey[1]; A. Kimura[2]; J. Farmer[1]; [1]Lawrence Livermore National Laboratory; [2]Kyoto University

Oxide Dispersion Strengthened (ODS) steels are primary candidate materials in fusion reactor cladding design due to their reduced activation, high temperature strength and creep resistance properties. The presence of nano-oxide features in ODS steels (typically Y2O3) is primarily responsible for this increased material performance. While experimental evidence indicates that these nano-oxides also act as sinks for Helium bubbles that form during exposure to neutron irradiation, and thereby improving swelling properties, it is not definitive due to the experimental restrictions (i.e. requirement to defocus in the TEM in order to observe voids). In this work, we present results from small angle X-ray scattering (SAXS) experiments performed at the Advanced Photon Source to characterize the nanofeatures present in ODS steels implanted with Helium ions. Two types of ODS steels were used in the study, each with differing nano-oxide size distributions, in order to observe how the oxide size distributions affect the resultant He bubbles. We also show that by taking advantage of operating the SAXS beamline in Anomalous mode (ASAXS), further elucidation of the Helium/nano-oxide structure is possible. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

3:40 PM Break

3:50 PM

Atomic Level Characterization of Advanced Radiation Tolerant Steels: *Michael Miller*[1]; D.T. Hoelzer[1]; K.F. Russell[1]; [1]Oak Ridge National Laboratory

The development of radiation tolerant materials for the next generation of advanced reactors requires state-of-the-art microstructural characterization tools to ensure that the microstructure remains stable during exposure to high doses of irradiation at elevated temperatures. Atom probe tomography permits atomic scale characterization of the size, composition, morphology, and number density of nanoscale precipitates as well as quantifying the levels and extent of solute segregation to grain boundaries and dislocations. Examples will be presented of the types of characterizations that are possible to perform on neutron irradiated nanostructured ferritic steels with a local electrode atom probe (LEAP®) in conjunction with a dual beam scanning electron microscope/focused ion beam milling system. This research was sponsored by the Division of Materials Sciences and Engineering and the SHaRE User Facility of the Scientific User Facilities Division in the Office of Basic Energy Sciences, U.S. Department of Energy.

4:10 PM Invited

The Corrosion of Oxide Dispersion Strengthened (ODS) Ferritic Steel in Molten Fluoride Salts: *Joseph Farmer*[1]; [1]Lawrence Livermore National Laboratory

Oxide dispersion strengthened (ODS) ferritic steel has exceptional high-temperature strength and swells very little during neutron irradiation. This material has already been successfully used as a cladding for high burn-up fission fuel, and is now being considered as a structural material for the construction of fusion, fission, and fusion-fission hybrid reactor systems. This material has been found to undergo corrosion in high temperature molten fluoride salts that may ultimately be used as coolants for fusion and fusion-fission reactor systems. Fluoride salts infiltrate the surface of the alloy, and preferentially dissolve chromium rich phases, as shown in scanning electron micrographs. A special high-temperature electrochemical cell has been developed that has enabled electrochemical impedance spectroscopy (EIS) to be performed at frequencies ranging from 0.001 to 500,000 Hz, and at temperatures of 800C to 1000C. This capability is being used to develop a detailed understanding of the corrosive attack of ODS steel by high temperature fluoride-salt coolants of importance to future generations of fusion reactors. Corrosion models have been developed that account for the frequency dispersion in the observed complex impedance, and have been compared to classic linear networks frequently used to interpret low-temperature impedance data. The techniques that have been developed have enabled in situ measurements of charge transfer kinetics, interfacial capacitance (double layer and passive film) and mass transport rates associated with corrosion. Corrosion resistant coatings for the protection of the ODS steel are also being investigated, and include alloys of tungsten, vanadium and nickel. Based upon thermo-chemical arguments, these materials should have some immunity to corrosion in such environments.

4:35 PM
Magnetic Environment-Dependent Migration Pathways of Point Defects in Fe-Cr Alloys: *Duc Nguyen-Manh*[1]; Mikhail Lavrentiev[1]; [1]UKAEA

In order to understand point defect properties generated under irradiation and to identify the kinetic pathways of micro-structural evolution in Fe-Cr system, a systematic density functional theory calculations of the activation energy of migration barriers for a vacancy jump at low-energy alloy configurations have been carried out using Nudged Elastic Band methods. We found by using spin-density maps at saddle point configurations that migration energy pathways are very sensitive to the magnetic behavior of the local atomic environments. A comparative study of vacancy migration pathways for modeling of phase separation in Fe-Cr binary using empirical inter-atomic potentials and conventional magnetic cluster expansion techniques demonstrates clearly the need of including of magnetic treatment which has been ignored in all previous kinetic Monte-Carlo simulations. We intend to use the created data base of magnetic environment-dependent migration energies to develop a new algorithm based on magnetic cluster expansion.

4:55 PM Invited
Tungsten-Rhenium Super Alloy Development for Ultra High Temperature Space Fission and Fusion Reactors: Jonathan Webb[1]; *Indrajit Charit*[2]; [1]Center for Space Nuclear Research; [2]University of Idaho

Tungsten based super alloys containing rhenium show great promise for uses in the space nuclear power and propulsion reactors as well as wall liners in fusion reactors. This paper will discuss previous research programs to develop and characterize tungsten-rhenium alloys and fuel forms. Different fabrication techniques will be discussed as well as material properties such as ductile to brittle transition temperature, tensile strength, super-plasticity and hardness. Historical methods of producing tungsten based fuel forms during the GE-710 and ANL nuclear rocket programs will be discussed as well as in core reactor testing at the Transient Test Reactor (TREAT) at the National Reactor Test Site in Idaho. Lastly a current program to develop tungsten-rhenium alloys at the Idaho National Laboratory along with the Center for Space Nuclear Research and the University of Idaho will be discussed.

5:25 PM Invited
Radiation Damage Study in Mo by in situ TEM/Ion Irradiation and Computer Modeling: *Meimei Li*[1]; Mark Kirk[1]; Pete Baldo[1]; Donghua Xu[2]; Thibault Faney[2]; Brian Wirth[2]; [1]ANL; [2]University of California

This paper presents the experimental data of radiation defects produced during in situ ion irradiation of pure molybdenum with 1MeV Kr ions at the IVEM-Tandem facility. In situ ion irradiation was carried out at 80 and 300C to a wide range of doses at dose rates over three orders of magnitude. Quantitative analysis was made to determine the number density and size distribution of defect clusters as a function of foil thickness, dose, dose rate and irradiation temperature. The experimental findings were compared with the computational data of defect cluster dynamic models using the rate theory. The identical material was previously neutron-irradiated at 80C in the HFIR. A direct comparison of defect microstructure was made to correlate damage between in situ ion and neutron irradiations. The findings showed that in situ ion irradiation provides valuable experimental data that can be used to benchmark computational modeling and simulate neutron damage.

5:55 PM Concluding Comments

Advances in Composite, Cellular and Natural Materials: Composites and Modelling

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS/ASM: Composite Materials Committee
Program Organizers: Yuyuan Zhao, The University of Liverpool; David Dunand, Northwestern University

Wednesday PM — Room: 305
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Larry Murr, University of Texas at El Paso; Martin Pech-Canul, Centro de Investigacion y de Estudios Avanzados del Instituto Politecnico Nacional

2:00 PM
An Accurate and Efficient Method for Constituent-Based Progressive Failure Modeling of a Woven Composite: *Ray Fertig*[1]; [1]Firehole Technologies

Accurate modeling of woven composites continues to challenge designers of composite structures. In order to make the problem computationally tractable, finite element modeling efforts usually require homogenization of the composite microstructure, which masks constituent interactions and stresses that actually drive failure. But because failure is a constituent level phenomenon, any general method for predicting initiation and propagation of failure must incorporate constituent behavior. In this paper we propose a computationally efficient method for failure prediction of a composite structure using finite element analysis. The approach requires using multicontinuum mechanics for a three-constituent composite to extract constituent-level stresses from a routine finite element analysis of a composite structure. Failure criteria are then applied at the constituent level to predict constituent failure, after which constituent and composite properties are adjusted. This technique is coupled with a numerically robust progressive failure algorithm to form a robust tool for failure prediction of composite weaves.

2:20 PM
Micro-Mechanical Modeling and Simulations Composites Using Reconstructed Three-Dimensional Microstructures: *Arun Gokhale*[1]; Arun Sreeranganathan[2]; Harpreet Singh[1]; Yuxiong Mao[1]; [1]Georgia Institute of Technology; [2]Stress Engineering Services Inc

Micro-mechanical response of composites depends on the morphology, anisotropy, and spatial arrangement of the reinforcement phase (particles, fibers, whiskers, etc.). Nonetheless, these aspects of the microstructural geometry are frequently ignored in the simulations of the mechanical behavior of composites. Further, most of the simulations are based on two-dimensional (2D) microstructures although real microstructures are three-dimensional (3D). In this contribution, we present simulations of the micro-mechanical behavior of real 3D microstructures of composites that utilize 3D volume segments of real microstructures. For this purpose, high resolution large volume segments of 3D microstructures are reconstructed. These 3D microstructure segments are implemented in the finite elements based simulations of the micro-mechanical response of the composites.

2:40 PM
Size Dependent Ductile Failure Analysis of Particle-Reinforced Composites via Finite Element Modeling of Dislocation Punched Zone: *Yeong Sung Suh*[1]; Yong Bae Kim[1]; Shailendra P. Joshi[2]; K. T. Ramesh[3]; [1]Hannam University; [2]National Singapore University; [3]Johns Hopkins University

A size dependent strength analysis of particle-reinforced composites via finite element modeling of augmented axisymmetric unit cell that includes dislocation punched zone by thermal mismatch between the particle and the matrix. Assuming that there is no particle fracture, the failure may take place either on the matrix-particle interface or in the matrix by ductile failure, depending on the particle size and the volume fraction. Initial study reveals this in such a way that the maximum plastic deformation is observed on the matrix-particle interface or inside the matrix adjacent to the punched zone. More in depth analysis that takes account of interface debonding and damage initiation and evolution in the matrix is in progress. It is expected to show that the failure of the particle-reinforced composites exhibits length scale according to the density of the geometrically necessary dislocations formed in the punched zone around the particle.

3:00 PM
SMT Reflow Jig Material Analysis: *Xin Ma*[1]; [1]Samsung Electronics (Suzhou) Semiconductor Co.Ltd / SESS

Nowadays, composite material is widely used in modern industries. In semiconductor industry, it has taken place of aluminium alloy gradually as surface mount technology (SMT) reflow jig material. The most wildly used composite material is scattering glass fiber composite material. But its structural defect is exposed during using. In this paper, the main factors leading failure of scattering glass fiber composite material have been analyzed; the finite element (FE) simulation has been done; and the improvement methods have been proposed. In addition, the thermal and mechanical properties have been tested and been compared with other two composite materials. Conclusion has been received that the composite material with glass fibers cross style waved can avoid the failure of scattering glass fiber composite material. Thus extend the service life of SMT reflow jig and decrease the misalign rate in solder print process.

3:20 PM
Microstructure in Work-Hardened Micro-Truss Materials Given Post-Forming Annealing Treatments: *Brandon Bouwhuis*[1]; Uta Klement[2]; Glenn Hibbard[1]; [1]University of Toronto; [2]Chalmers Institute of Technology

Micro-truss cellular materials can be used as structurally efficient cores in light-weight sandwich panels. These sandwich cores have been produced using deformation-forming approaches, which introduce plastic strain into the truss struts. While this imparted strain can be used to strengthen the overall micro-truss core, it also drives recrystallization and grain growth if sandwich panel assembly involves conventional brazing treatments that subject the truss core to elevated temperatures. In addition to losing a potential strengthening mechanism, brazing can also result in the grain size of the annealed microstructure approaching the cross-sectional dimensions of the micro-truss struts. The present study is an examination of the strut microstructures in aluminum alloy and stainless steel micro-truss materials fabricated using a deformation-forming approach, and following a post-fabrication annealing step. These results serve as a guideline for future sandwich panel thermal processing to minimize the reduction of strength due to annealing and detrimental size effects.

3:40 PM Break

4:00 PM
Wear Behavior of SiC /Al-Si Alloy Matrix Composites Produced by Squeeze Casting: *Muna Abbass*[1]; [1]University of Technology, Baghdad

The aim of present work is to study dry sliding wear behavior of the (Al – 12 % Si) matrix alloy reinforced with 5wt% SiC particles. Composite materials were prepared by stir casting using vortex technique and squeeze casting under varying casting pressures from 7.5 to 53 MPa , and mold preheating at temperature (200oC). Microstructure and hardness for prepared composite materials were carried out. Wear tests of type (Pin–on-Disc) were conducted at varying loads from 5 to 20 N under a constant sliding speed of 2.7 m / sec. The results showed that a refinement in the microstructure with increasing the squeeze pressure. Increasing the squeeze pressure resulted in increasing the hardness and decreasing the wear rate. It has been found that the composites produced by squeeze casting have wear resistance higher than that of the stir casting.

4:20 PM
Influence of Heating of Al2O3 Particle with Holding Time Variation to Compactibility of Al/Al2O3 Isotropic Composite: *Widyastuti*[1]; Mochamad Zainuri[1]; Agita Riani[1]; [1]ITS Surabaya

Heating of Al2O3 particles is one of the ways to increase the quality of the bonding. In this research, volume fraction Al2O3 are 10, 20, 30, 40% heated on 1100°C and hold on 2, 4, 6 hours. Then, Al and Al2O3 are mixed and compacted by 25kN for 15 minutes. Pre sintering temperature is 200°C for 30 minutes and sintering temperature is 600°C for 2 hours. The result shows that the increasing volume fraction will increase modulus elasticity on 2 and 4 hours but decrease it on 6 hours. The increasing holding time will decrease the value of modulus elasticity. The best volume fraction and holding time of heating process are 40% and 2 hours.

4:40 PM
Effect of Vacuum Degassing on Composites Preparation: *Che Dehui*[1]; Yao Guangchun[1]; Kang Wei[1]; Zhang Xiaoming[1]; [1]Institute of Materials and Metallurgy, Northeastern University

In processing of preparation of carbon fiber reinforced aluminum matrix composite materials by stirring casting and a vacuum degassing process was used after mixing. The porosity of the composite materials is effectively reduced and therefore the mechanical properties of composites are enhanced. In this paper, the carbon fiber-reinforced A356 alloy matrix composite slurry was degassed in 0.2 Pa vacuum, and the effect of temperature and time on the density of composites were studied. When the temperature is 700°C, degassing 2 min, the porosity of composites reduced to 0.2%. And interface morphology of the composites was characterized by SEM and no hole was found.

5:00 PM
Fabrication of Carbon Nanotube Grown on Al Powders Reinforced Al Matrix Composite: Chitoshi Masuda[1]; *Fumio Ogawa*[2]; Ryoichi Hirashima[2]; [1]Waseda University; [2]Graduate School of Waseda University

Carbon nanotubes have very high strength and physical properties. For fabrication of carbon nanotube reinforced composites the agglomeration of carbon nanotubes are very big problem to distribute homogeneously in the matrix. To improve the agglomeration of carbon nanotubes, the carbon nanotubes are grown on the metal powders and mixed with metal powers.In this presentation the carbon nanotubes are tried to be grown on Al powders by CVD method. On the Al powders (average size is about 17μm in diameter) are used and carbon nanotubes are grown in the vaccum chamber by alcohol atmosphere. The fine carbon nanotubes were grown on the Al powders. The diameter of CNT is about 30nm and its length is about 10μm. The Al powders grown by CNT were consolidated by SPS method. The mechanical properties of balk materials were examined. Moreover, the grown CNTs were checked by TEM and EDX.

5:20 PM
Diffusion of Liquid Media in Vulkanizats: *Milena Milenova*[1]; Verjinia Aleksandrova[1]; Aleksandar Aleksandrov[1]; Gunai Halil[1]; [1]University of Chemical Technologi and Metallurgy- Sofia

The kinetics of the diffusion of aggressive, liquid and industrial mediums in vulcanizers are concerned in the present study in view of further investigation of the influence of diffusion on their deformation and strength characteristics. The penetration is realized through a diffusion i.e. the liquid migrates in the body's volume under the influence of the concentrative gradient. The distribution of the diffunding liquid's concentration in the different points of the body can be described by the so called Fick's second law. The solution depends on the body's form and the initial and border conditions of the particular problem and it is based on the concept average concentration. In our case the calculations showed that for different average concentrations, the diffusion coefficient may vary within close limits and with a sufficient for the engineering practice it may be accepted as a constant.

Alumina and Bauxite: Bauxite Characterization and Handling

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee, TMS: Aluminum Processing Committee
Program Organizers: Carlos Suarez, Hatch Associates Inc; Everett Phillips, Nalco Company

Wednesday PM — Room: 612
February 17, 2010 — Location: Washington State Convention Center

Session Chair: Jorge Aldi, Alunorte

2:00 PM Introductory Comments

2:10 PM
Reduction Roasting and Fe-Al Separation of High Iron Content Gibbsite-Type Bauxite Ores: *Guanghui Li*[1]; Na Sun[1]; Jinghua Zeng[1]; Zhongping Zhu[1]; Tao Jiang[1]; [1]School of Minerals Processing & Bioengineering; Central South University

Large reserves of high iron gibbsite-type has been found in China, which is characterized as relatively high iron content, but low alumina content and A/S ratio. Aluminiferous minerals and ferrous minerals are fine or superfine in size, and conjoint and substituted with each other; therefore, physical beneficiation is impracticable due to extremely difficult liberation. In this study, reduction roasting and separation of iron and aluminum has been investigated. The influences of reduction time, roasting temperature and magnetic separation were involved. The results indicate that when process a sample with 31.22% total iron grade and 26.35% alumina, a metallic iron concentrate with 93.3% total iron grade and non-magnetic product with 40% alumina content were obtained. Metallic iron concentrate can be used as steelmaking burden, and alumina can be extracted from the non-magnetic product further.

2:40 PM
Study and Application of an Improved Sintering Process with Pre-Drying of Raw Material Slurries: *Hengqin Zhao*[1]; Baozhong Lu[2]; Hualong Ma[1]; [1]Zhengzhou Institute of Multipurpose Utilization of Mineral Resources, CAGS; [2]Shanxi Zhongke PACL Co. Ltd

An improved sintering process to produce alumina was studied. The raw material slurries with proper mass ratio were dried with waste gas of kiln. The temperature of waste gas of kiln was decreased to under 110°C from above 500°C during drying of the slurries. The content of moisture of the slurries was reduced to 5% from 40% through drying process with the waste gas of the kiln. The dried slurries called as dry raw slurries were fed to the kiln and were sintered to the sinter. The aluminate sodium of the obtained sinter was very easy to be leached and leaching rate of alumina and oxide sodium in the obtained sinter reached to up 90% and 95% respectively. According to industrial application after adoption of the improved sintering process, consumption of coal in the sintering can be decreased by 18% than before improvement.

3:10 PM
Bayer Process and Soda-Lime Sintering Process of Special Diasporic Bauxite with High Silica: *Cao Wenzhong*[1]; Tian Weiwei[1]; Shong Hong[1]; [1]Environmental and Chemical Engineering Institute, Nanchang University

The bauxite in the eastern region of China is diasporic type with high silica containing about 8-16% SiO2. The main silica minerals in the bauxite are kaolinite, chamosite and illite. Technological investigations were carried out based on the Bayer process and a soda-lime sintering process. Sintering and leaching properties of the clinker in the sintering process, and the settling characteristics of the red mud were determined. The presence of high silica causes high bound-soda losses in the red mud in the Bayer process, though a part of silica content in the bauxite was in the form of chamosite. However, the bound-soda losses can be greatly reduced by using soda-lime sintering process. Therefore, it is necessary to study Bayer process, sintering and leaching properties of the special diasporic bauxite with high silica.

3:40 PM Break

4:00 PM Discussion Time

Alumina and Bauxite: Industry Trends and Issues

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee, TMS: Aluminum Processing Committee
Program Organizers: Carlos Suarez, Hatch Associates Inc; Everett Phillips, Nalco Company

Wednesday PM February 17, 2010
Room: 611
Location: Washington State Convention Center

Session Chair: Benny Raahauge, FLSmidth Denmark

2:00 PM Introductory Comments

2:10 PM
Heat Transfer in the Bayer Process: *Daniel Thomas*[1]; Michael Evans[1]; [1]WorleyParsons

Heat transfer equipment represents a significant portion of Bayer process plant capital and operating costs. Heater operation and maintenance activities can also create potential hazard exposure. Very early flowsheets tended to rely on batch operation and/or direct heat transfer (steam injection), and this still persists to some extent today. There has however been an ever increasing utilisation of indirect heat exchange over the past 100 years. This has been driven by higher energy costs and enabled by improved heat transfer equipment. This paper presents an historical perspective, explores some heater selection case studies, and looks at future challenges and opportunities.

2:40 PM
Sustainable Bauxite Mining - A Global Perspective: Christian Wagner[1]; Bauxite & Alumina Committee of the International Aluminium Institute[1]; [1]International Aluminium Institute

In 2008 the International Aluminium Institute commissioned its fourth sustainable bauxite mining report with the aim to collect global data on the environmental, social and economic impacts of bauxite mining operations and their rehabilitation programmes. The report shows that bauxite mining has become sustainable and land area footprint neutral; it is a relatively small land use operation when compared to most other types of mining. All operations have clearly defined rehabilitation objectives, fully integrated rehabilitation programmes, and written rehabilitation procedures. Almost 80% of the surveyed mines are ISO 14001 certified for environmental management. Bauxite miners are actively engaging with local communities to support development through employment, infrastructure, training and social programmes and compensatory packages. Displacement and resettlement issues are limited for the bauxite mining industry in total, but of high priority at the individual level for the people that need to be displaced and relocated.

3:10 PM Break

3:30 PM
The Need for Energy Efficiency in Bayer Refining: *Lawrie Henrickson*[1]; [1]WorleyParsons

During the recent economic boom, the high Alumina price encouraged rapid expansion of world Alumina refining capacity. The main objective was speed rather than efficiency, so refineries were constructed faster than ever before, especially in China, taking advantage of lucrative profit margins, without much concern for operating cost. However, when the world economy crashed in late 2008, the fall in commodities prices caused a severe profit squeeze at many refineries. The lack of built-in efficiency caused many refineries to wind-back production or commence full shut-down. The main operating cost pressure was energy, even with much lower unit energy costs. This paper examines the key energy efficiency drivers for a refinery, and evaluates the trade-off of capital cost against operating cost, with the expectation of rising long-term energy prices. The option of Brownfields retrofits against Greenfields installations is also discussed.

4:00 PM
A Case for Replication of Alumina Plants: *Anthony Kjar*[1]; [1]Gibson Crest Pty Ltd

Rising capital costs of one off greenfield projects in many countries as well as a stalled creep capacity increase is a rate limiting step for many alumina producers. A new approach is required to enable Western alumina producers to develop in an economic way increased capacity to match rising demand and not loose further market share to Chinese producers. There are leassons to be learnt from a replication approach. This has been successful for periods of time in gold, coal processing, power stations, and is now being tried in copper processing, nuclear power reactors and in many Chinese developments in nickel, magnesium and aluminium.

Aluminum Alloys: Fabrication, Characterization and Applications: Emerging Technologies

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Processing Committee
Program Organizers: Subodh Das, Phinix LLC; Steven Long, Kaiser Aluminum Corporation; Tongguang Zhai, University of Kentucky

Wednesday PM Room: 615
February 17, 2010 Location: Washington State Convention Center

Session Chair: Subodh Das, Phinix LLC.

2:00 PM
Microstructure of Ultrasonic Impact Treated Aluminum 5456-H116: *Kim Ngoc Tran*[1]; Elissa Bumiller[1]; Lourdes Salamanca-Riba[2]; [1]Naval Surface Warfare Carderock Division; [2]Univeristy of Maryland

The Navy is using ultrasonic impact treatment (UIT) experimentally to treat 5456-H116 in order to mitigate crack initiation and propagation. While UIT has been shown to be promising, the effects of UIT on the properties and microstructure of 5456-H116 are not understood. The Navy is investigating the effects of UIT on 5456-H116 through material characterization and material's property testing. The objective of the work is to develop a fundamental understanding of the mechanisms that cause material property changes. Preliminary work to characterize UIT treated plate is in progress. This work includes x-ray diffraction measurements, surface profilmetry, optical microscopy (OM), scanning electron microscopy (SEM) combined with electron backscattering diffraction, and tensile testing. Current work expands the scope to include the evaluation of treated welds. This work includes transmission electron microscopy (TEM), in-situ TEM using a heating stage, ASTM-G67 testing for intergranular corrosion, nanohardness measurements, additional mechanical testing, OM, and SEM.

2:20 PM
Charge Weld Effects in High Cycle Fatigue Behavior of a Hollow Extruded AA6082 Profile: *Nicholas Nanninga*[1]; Calvin White[2]; [1]NIST; [2]Michigan Technological University

Fatigue properties of specimens taken from different locations along the length of a hollow AA6082 extrusion where charge weld properties and the degree of coring are expected to vary have been evaluated. The fatigue strengths of transverse specimens containing charge welds are lower near the front of the extrusion where the charge weld separation is relatively large. The lower fatigue properties of the AA6082 specimens appear to be associated with early overload fatigue failure along the charge weld interface. Coring does not appear to have significantly affected fatigue behavior in either of these alloys.

2:40 PM
Ag Nanoparticles Dispersion on Surface-Modified Al Alloy Porous Body and Their Filtration Properties: Young Ik Seo[1]; Se Hwan An[1]; Dae-gun Kim[1]; Kyu Hwan Lee[2]; *Young Do Kim*[1]; [1]Hanyang University; [2]Korea Institute of Science and Technology

For the water purification and anti-bacterial filters, the combination of the enlarged specific surface area and anti-microbial material is necessary for the filtration efficiency. Because the pore surface acts as an adsorption site with impurities and the anti-microbial material, such as silver nanoparticle, suppresses the proliferation of bacteria. Silver nanoparticle dispersed Al-4wt.% Cu porous body was manufactured by the following manner. The granulated powder was fabricated by low energy ball mill and was compacted under the pressure of 20 MPa for macropore network. After sintering, the sintered body was surface-modified in dilute alkali solution for microporous surface. Subsequently, the surface-modified porous body was immersed in the solution that was synthesizing Ag nanoparticles by polyol process. The scanning electron microscopy (SEM) and transmission electron microscopy (TEM) were employed to investigate the microstructure and phase confirmation. Permeability and filtration characteristics evaluated by specially manufactured device using pure water and artificial waste water.

3:00 PM
Incubation Behavior of Hg-LME in Aluminum: Scott Keller[1]; *Ali Gordon*[1]; [1]University of Central Florida

When high strength aluminum alloys are subjected to liquid metals, physical and chemical reactions ensue resulting in what is known as liquid metal embrittlement (LME). A subset of stress corrosion cracking, LME is exhibited when a liquid metal, e.g. Hg or Ga, comes into intimate contact with a solid metal having significant susceptibility. As mechanical loads are applied, the interaction between the two metals results in a reduction in the flow properties of the solid metal. Several theories have been proposed to identify the underlying microstructural failure mechanism; however, none have been widely accepted. Crack growth experiments on Al 7075–T651 in liquid mercury have been conducted to extend these physically-based theories. Through constant stress intensity factor (SIF) tests, incubation periods were analyzed, providing data for a diffusion-based theory of LME. These mechanical test data, along with metallographic analysis, show that the phenomena of LME is both strongly time- and SIF-dependent.

3:20 PM
Recent Advances in FSW Joining of Sheets on Structural Extruded Profiles: *Lorenzo Donati*[1]; [1]University of Bologna

Recently industries involved in train, airplane and ship construction increased the use of FSW for replacement of traditional assembly technologies like mechanical fasteners (bolts and rivets) and MIG or TIG welding. The FSW technology is usually applied in joining two sheets in the butt joint configuration. Nevertheless, some industrial applications require the joining of three bodies, usually called T-joint or corner welds. In this work a detailed study on the union of two sheets on an extruded structural profile is presented. The innovative idea presented is related to the opportunity of freely shaping the extruded profile, thus allowing the production of appendix suitable to be used as filler material or clamping system during the FSW stage. Three types of profile shapes were used (simple, with I and T appendix) and, for each condition, optimizations of PIN shape and process parameters were carried out based on tensile tests and microstuctural analysis.

3:40 PM Break

3:55 PM
Adiabatic Shear Localization of Al-Sc Alloy at Extremely High Strain Rates: *Woei-Shyan Lee*[1]; Tao-Hsing Chen[2]; Ging-Ting Lu[1]; [1]Department of Mechanical Engineering, National Cheng Kung University; [2]Center for Micro/Nano Science and Technology, National Cheng Kung University

The adiabatic shear behaviour of aluminum-scandium(Al-Sc) alloy under high strain rates ranging from 3.0×105 s-1 to 6.3×105 s-1 is studied by using a compressive-type split-Hopkinson pressure bar (SHPB). The results show that both the shear stress and the strain rate sensitivity increase with increasing the strain rate. In addition, it is shown that an adiabatic shear band is formed within the deformed specimens for all values of the strain rate. As the strain rate is increased, the width of the shear band decreases, but the microhardness increases. At a strain rate of 3.0×105 s-1, the fracture surface is characterised by multiple transgranular cleavage fractures. However, for strain rates greater than 4.5×105 s1, the fracture surface has a transgranular dimple-like characteristic, and thus it is inferred that the ductility of the unweldable Al-Sc alloy improves with increasing the strain rate.

4:15 PM
Effect of Electric Potential on the Evolution of Defect Substructure and Fracture Surface of Aluminum under Creep: Sergey Konovalov[1]; Oksana Stolboushkina[1]; Yurii Ivanov[2]; Roman Filipiev[1]; *Viktor Gromov*[1]; [1]Siberian State Industrial University; [2]Institute of High Current Electronics Siberian Brach of Russian Academy of Science

The investigation of the morphology of the fracture surface and defect substructure, which is formed with creep in the zone of the fracture of the samples of technical pure aluminum are carried out by the methods of scanning and diffraction electron microscopy. It is shown that the structure, which is formed under creep conditions under the potential, is characterized by the higher degree of self-organizing dislocation substructure in the zone of the fracture of samples, in comparison with the samples, destroyed with creep under the normal conditions.

Wed. PM

4:35 PM
Using Artificial Neural Network to Optimize the Bakehardening of AL2024 and AL7075: *Niloofar Kamkar Zahmatkesh*[1]; Kamran Dehghani[1]; Atiyeh Nekahi[1]; [1]Amirkabir University of Technology

In the present work, the response of two aluminum alloys (Al2024 and Al7075) to strain aging and bake hardening (BH) was investigated. After the primary heat treatments, the direct chilled ingots were subjected to laboratory cold rolling. Various treatments and different testing conditions were used to evaluate the aging and baking behaviors of the mentioned alloys. The different strains were applied so that to attain different dislocation densities required for attaining various aging and baking values. The results show that the higher the strain, the greater the strain aging and bake hardening amounts will be. Experimental data was used for the training of ANN and a multilayer cascade forward back-propagation neural network was designed. The optimization was achieved by minimizing the errors between the predicted values and the ones that were obtained experimentally. The predicted values obtained from the trained ANN are found to be in close agreement with the experimental results.

4:55 PM
Defects Producing Formation of Microcracks in Aluminum during Electrochemical Charging with Hydrogen: *Paul Rozenak*[1]; [1]Hydrogen Energy Batteries LTD

The formation of micro-cracks in high purity aluminum during electrochemical charging by hydrogen was studied. The experiments reveal that, in aluminum samples, a wide distribution of hydrogen bubbles on the surface (blisters) and under the surface into the volume, were produced during electrochemical charging. This phenomenon can lead to the formation of micro-cracks in the absence of externally applied stress. Examination of electrochemically charged samples by transmission electron microscopy (TEM) showed micro-cracks with a typically ductile mode of fracture.

Aluminum Reduction Technology: Hall-Héroult Cell: Process Control

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee, TMS: Aluminum Processing Committee
Program Organizers: Charles Mark Read, Bechtel Corporation; Gilles Dufour, Aluminerie de Deschambault

Wednesday PM — Room: 608
February 17, 2010 — Location: Washington State Convention Center

Session Chair: Alan Phillips, KTD LLC

2:00 PM Introductory Comments

2:10 PM
Continuous Improvement in Aluminium Reduction Cell Process Performance with the ALPSYS® Control System: *Sylvain Fardeau*[1]; Benoît Sulmont[1]; Philippe Vellemans[1]; Claude Ritter[1]; [1]Rio Tinto Alcan

Improving cell productivity through increased current generally leads to higher anode current densities, lower bath to amperage ratios and changed cell dynamics. Up-to-date process control is required in order to maintain or improve existing performance under these increasingly challenging conditions. The ALPSYS® control system has been continuously improved to cope with these new constraints. It provides innovative solutions in order to increase cell productivity while moving towards zero anode effects.This paper shows how a large scale deployment of the latest alumina control developments has resulted in a significant reduction of anode effect rate while increasing cell productivity in the Alma smelter. It also shows how the sharing of best practices for anode effect treatment has enabled a halving of anode effect duration in all Alcan AP plants. Hence, even for benchmark cell technology, effective process control can further improve current efficiency while reducing green house gas emissions.

2:40 PM
A Nonlinear Model Based (NMPC) Control Strategy for the Aluminium Electrolysis Process: *Steinar Kolas*[1]; Stein Wasbø[2]; [1]Hydro; [2]Cybernetica AS

Important factors for the aluminium industry for succeeding in reducing greenhouse gas emissions and increase energy efficiency is not only the speed in which the organization is able to utilize new knowledge, but also the development and use of new advanced process control systems. New advanced process control systems imply utilizing state of the art process control systems as e.g. Nonlinear Model Predictive Control (NMPC). Although the conventional control structures are dominating the aluminium industry, several authors have addressed advanced process control structures for controlling the Hall-Heroult process. This includes the adaptive control of alumina addition, 9 -Box Matrix Control, LQG Control, Model Predictive Control and control structures involving the Neural network approach. Recently Hydro has been active in developing an NMPC control structure for controlling the Hall-Heroult process. The Hydro NMPC control structure and results from operational practice on Hydro's Hal4e cells is presented.

3:10 PM
CVG-Venalum Potline Control and Supervisory Integrated System VEN-PCSIS: *Jose Ramones*[1]; Frangil Ramirez[1]; María Colmenares[1]; Jesus Larez[1]; Jesus Gonzalez[1]; [1]CVG Venalum

Profitability of smelters strongly depends on cells performance; therefore efforts are dedicated into increasing production capacity, reducing energy consumption, shifting from raw material providers, testing new anode or cathode designs, and so on. To successfully accomplish these changes, as well as the necessary adjustments on pot operations, companies must be capable of developing control and supervisory systems to handle such challenges. Friendly human machine interface satisfying information handling requirements from cell operators is also needed, so strict monitoring of cells performance can be easily performed on real time. To fulfill these targets, CVG-Venalum developed an aluminum reduction pot control and supervisory integrated system (VEN-PCSIS). The central control unit of VEN-PCSIS is based on a PC-104 standard board, and the supervisory system runs on free-software web technology. Results of VEN-PCSIS during the trial period overpowered existing systems; hence CVG-Venalum management decided replacing former cell control and supervisory systems with the VEN-PCSIS.

3:40 PM Break

3:50 PM
Efficient Thermal Balance Strategy Developed by CVG Venalum: *Maria Colmenares*[1]; Adela Ruiz[1]; Jesus Imery[1]; [1]CVG Venalum

Worldwide, in order to keep their businesses as profitable as possible, smelters are aware of the key importance of improving any aspect of their processes, whilst increasing production capacity. This never ending quest, in many cases brings cells at or beyond their former performance limits, which strongly impacts the thermal balance. As a result, developing a control strategy capable of dealing with managerial targets, and yet successfully minimizing bath temperature deviations with a minimum consumption of aluminum fluoride became a very desirable asset. This paper describes the development of a temperature control system using fuzzy logic algorithms. Results obtained during the stage trail in three different aluminum reduction cell technologies were outstanding, with a significant reduction in bath temperature and bath acidity deviations with reduced aluminum fluoride consumption. Nowadays, the system is operating in most of the 905 cells of CVG –VENALUM

4:20 PM
Usage of Fuzzy Logic as a Strategy for the Aluminium Fluoride Addition in Electrolytic Cells: *Fabio Soares*[1]; [1]Exodus

This work describes an Intelligent Aluminum Fluoride (AlF3) Addition Strategy in Electrolytic Cells, based on Fuzzy Logic concepts, wherein the knowledge retained by process specialists is qualitatively translated into a set of linguistic rules such as: IF < condition > THEN < action >. The usage of a Fuzzy Strategy is justified by its natural capacity of dealing with inaccurate information, along with the absence of a known available dynamic model which takes into account the knowledge acquired by process specialists in Albras for each Cell, instead of using classical methods for modeling the process whose great complexity of the thermodynamic and electromagnetic phenomena involved is a very awkward problem

4:50 PM
Development and Application of a Multivariate Process Parameters Intelligence Control Technology for Aluminum Reduction Cells: *Yi Xiaobing*[1]; Tian Qinghong[1]; [1]CHALIECO

Everybody knows that the aluminum reduction process has strong interaction multivariate characteristics with limited process observability and responses which are non-linear and vary over a wide range of time scales. Generally saying, the process and control technology developed and used in each aluminum smelter worldwide, which are based on different control philosophy, normally are different from others. This paper emphasizes on the introduction of one advanced multivariate process parameters intelligence control technology developed by CHALIECO GAMI in recent years, and its successful application resulting in significantly higher current efficiency and reduced energy consumption by several large domestic and abroad green-field or modernized smelters.

5:20 PM Concluding Comments

Biological Materials Science: Surface Engineering: Biomimetics and Biological Applications

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS: Biomaterials Committee, TMS/ASM: Mechanical Behavior of Materials Committee
Program Organizers: John Nychka, University of Alberta; Jamie Kruzic, Oregon State University; Mehmet Sarikaya, University of Washington; Amit Bandyopadhyay, Washington State University

Wednesday PM Room: 205
February 17, 2010 Location: Washington State Convention Center

Session Chairs: Marc Meyers, UCSD; Devesh Misra, University of Louisiana

2:00 PM Invited
Oxide Wettability: Jim Ruud[1]; *Molly Gentleman*[2]; [1]GE Global Research; [2]Texas A&M University

Oxides are believed to be hydrophilic because of the strong affinity for hydroxylation at their surfaces. This paper explores the relationship between hydroxylation of oxide surfaces and their resulting wettability. Here we demonstrate that hydroxyls increase the hydrophobicity, or reduce the wettability, of oxide surfaces by reducing the polar component of surface free energy. Using alumina as a model material, increased hydrophobicity with hydroxylation was confirmed experimentally and a correlation between the strength of the hydroxyl-driven hydrophobic response and surface treatment was demonstrated. Additionally an overview of how to design oxides with increased hydrophobicity will be discussed.

2:30 PM
In situ Biomimetic Ceramic Coatings: Jadid Samad[1]; *John Nychka*[1]; [1]University of Alberta

Biomimetic approaches for the creation of hydrophobic surfaces has generally, like nature, focused upon altering surface morphology to effect changes in wettability. The wetting angle of liquids on solid surfaces depends on rather few variables and nature has optimized the morphology of surfaces, along with their chemistry, to achieve incredible hydrophobicity -recall the lotus leaf. We report on our method to alter the wettability of surfaces of metallic substrates through creation of in situ oxide layers of varying morphology via simple oxidation treatments in air. Changes in wetting angle from over 100 degrees to less than 40 degrees can be achieved through such simple treatments.

2:50 PM
Surface Modification of Laser Processed Nitinol: *Sheldon Bernard*[1]; Susmita Bose[1]; Amit Bandyopadhyay[1]; [1]Washington State University

Nitinol (NiTi) is an equiatomic intermetallic compound of nickel and titanium whose unique mechanical properties contribute to its increasing use as a biomaterial. The objective of this research is to modify the surface of laser processed NiTi via anodization to enhance biocompatibility. Laser Engineering Net Shaping (LENS™) processed fully dense NiTi (50/50 atom%) samples were anodized in 1N sulfuric acid (H2SO4) electrolyte at three different pHs, 4.5, 2.0 and 1.5. All anodization experiments were performed at 20V and 30°C. Using anodization, we were able to improve the surface wettability by lowering the contact angle from 32 degrees to less than 5 degrees. The surface free energy was also calculated to show comparable properties to that of cpTi. This presentation will focus on influence of surface morphology on wettability, surface free energy, bone cell-materials interactions and Ni ion release of LENS™ processed NiTi.

3:10 PM
Grain Boundary Grooving and Its Effect on Biological Response: *Wah Wah Thein-Han*[1]; Devesh Misra[1]; Mahesh Somani[2]; Pentti Karjalainen[2]; [1]University of Louisiana; [2]University of Oulu

Metallic materials with sub-micron to nanometer-sized grains provide surfaces that are different from conventional polycrystalline materials because of the large proportion of grain boundaries with high free energy. Grooving of grain boundaries is expected to stimulate biological response. In this regard, we describe the cellular response of grooved grain boundaries in nanograined/ultrafine-grained materials. The improved cellular response is described in terms of initial cell attachment, proliferation, viability, morphology and spread on the nanograined/ ultrafine-grained grooved surface. Furthermore, grooving of grain boundaries demonstrated superior biological properties in terms of immunocytochemistry and protein analysis compared to the ungrooved substrate.

3:30 PM
Interaction of Ti-Fe Based Alloys with L929 Cells: *Arnaud Caron*[1]; Dmitri Louzguine-Luzgin[2]; Franz-Günter Sander[3]; Akihisa Inoue[2]; Hans-Jörg Fecht[1]; [1]Institute of Micro- and Nanomaterials, University Ulm; [2]WPI Advanced Institute for Materials Research, Tohoku University; [3]Department of Orthodentics, University Ulm

Mechanical testing of Ti-Fe based alloys reveal outstanding properties. In this work we investigate the toxicity of this alloy class on L929 cells by direct cell contact and filter test. These tests give good prediction on the ability of the alloys to be used as dental implants. Before and after toxicity tests, the alloy samples are investigated by scanning electron microscopy and atomic force acoustic microscopy in order to investigate eventual corrosion events on the samples surface after testing.

3:50 PM Break

4:00 PM
Bone Cell Infiltration in Porous Graphitic Surfaces: Influence of Surface Coatings and Nanotube Grafting: *Sharmila Mukhopadhyay*[1]; Elizabeth Maurer[1]; Saber Hussain[2]; [1]Wright State University; [2]Air Force Research Laboratory

This investigation aims at understanding the interaction of bone cells with graphite, and the possibility of enhancing their growth into porous scaffolds by surface modification. Graphitic foam samples having interconnected porosity, low density, and controllable thermal and electrical properties have been used for attachment and growth of osteoblast cells. The influence of surface coatings such as collagen and silica has been studied. Additionally, carbon nanotubes have been grafted on these substrates and the subsequent adhesion and proliferation of bone cells through these hierarchical porous structures has been investigated. Biocompatibility studies are done by various cell staining and imaging techniques, as well as mitochondrial functionality assays. Structural and functional evaluation of carbon-bone composites are performed using microscopy, spectroscopy, mechanical and electrical tests. These results indicate that the proliferation and overall functionality of bone cells in porous graphitic scaffolds can indeed be controlled, and significantly improved for use in future implant materials.

4:20 PM
Bovine Serum Albumin Protein Adsorption and Release on Electrically Polarized Biphasic Calcium Phosphates: *Mohammad Tarafder*[1]; Subhadip Bodhak[1]; Shashwat Banerjee[1]; Amit Bandyopadhyay[1]; Susmita Bose[1]; [1]Washington State University

Calcium phosphates (CP) are widely used in bone tissue engineering due to their compositional similarity with human bone. Our objective here is to investigate adsorption and release behavior of bovine serum albumin (BSA) as a model protein on the positively and negatively poled surfaces of three different biphasic calcium phosphate (BCP) composites. Three different biphasic calcium phosphate composites with different weight percent ratio of hydroxyapatite and ß-tricalcium phosphate were prepared and then polarized.

Stored charge density showed the increasing trend with the increasing percent content of HAp in the composites. Bovine serum albumin protein adsorption on the positively-poled surfaces was maximum after 6-hour. BSA release from the positively-poled surfaces was performed for up to 48-hour at 7.4 pH. A decreasing trend in percent release of BSA was observed with the increasing charge density. The presentation will discuss processing and characterization of BCPs and BSA adsorption and release behavior from them.

4:40 PM
Magnetic Nanoparticle Interactions with Hydroxyapatite: *Otto Wilson*[1]; Meron Haimanot[1]; [1]Catholic University of America

Enhanced functionality can be imparted to biomaterial implants at the macroscale, microscale, or nanoscale level and can involve a multitude of features related to bioactivity. These factors work together to orchestrate cell function, overall tissue healing, and promote seamless integration of the biomaterial implant into the neighboring tissue. Magnetic nanoparticles (MNPs) were adsorbed onto nanophase hydroxyapatite (HAp) particles to develop magnetically active hydroxyapatite. MNP modified HAp particles were characterized via electrophoretic mobility, particle size ananlysis, and electron microscopy. The MNPs rapidly adsorbed onto the surface of the HAp via heterocoagulation based interactions. MNP surface modification of HAp imparts magnetic behavior and allows the HAp to be translated in solution via magnetic fields. Applications for this novel HAp in hard tissue engineering will be presented with a focus on mechanically stimulated scaffolds for enhanced cell activity.

5:00 PM
Solid-Binding Peptide-Based Antibacterial Implants: *Hilal Yazici*[1]; Mary Rood[1]; Brandon Wilson[1]; Mustafa Gungormus[1]; Candan Tamerler[1]; Mehmet Sarikaya[1]; [1]University of Washington

Implant-associated infections are a primary cause of early implant failures. Prescribed oral antibiotics are not always effective because of the inability to reach the infection site and an increase in bacterial resistance. A novel class of peptides, the antimicrobial peptides (AMPs), is useful mainly because of the difficulty for microorganisms to develop resistance towards them. In the present study, we use a novel bi-functional peptide based approach that exhibits both titanium-binding (TiBP1) antimicrobial (AMP) properties for implant surface functionalization. The efficiency of TiBP1-AMP bi-functional was evaluated both in solution by analyzing bacterial growth using optical density measurement and on the functionalized titanium surface with fluorescence microscopy, scanning electron microscopy analysis at various time points. For example, Streptococcus mutans adhesion was reduced on the TiBP1-AMP peptide-based functionalized substrate compared to controls. The approach may be a candidate for the prevention of implant infections. This research is supported by GEMSEC at UW.

5:20 PM
Development of Anti-Microbial Silver Coating on Stainless Steel: *Paul DeVasConCellos*[1]; Susmita Bose[1]; Amit Bandyopadhyay[1]; Lewis Zirkle[2]; [1]BRC, Washington State University; [2]Surgical Implant Generation Network (SIGN)

Silver has been utilized for many years as an antimicrobial agent. With an increasing amount of antibiotic-resistant bacteria, silver-coatings and treatments are again being noticed as an effective way to prevent infection. In situations where cost effectiveness is necessary, the use of silver coatings on medical implants could be a valuable addition to help prevent infections. This is especially crucial when surgeries are performed in environments where sanitation is not ensured as well as environments in North American Hospitals. This research presents methods and feasibility of silver coatings on stainless steel (SS) which is a practical material for low cost implants. There are many parameters that can be adjusted for each method to apply silver coatings. In an effort to optimize antimicrobial effectiveness and keep human cell-toxicity to a minimum, we have experimented with various coating parameters and observed their effects on the utility of silver coating on SIGN SS-implants.

Bulk Metallic Glasses VII: Simulation and Modeling

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee
Program Organizers: Peter Liaw, The University of Tennessee; Hahn Choo, The University of Tennessee; Yanfei Gao, The University of Tennessee; Gongyao Wang, University of Tennessee

Wednesday PM February 17, 2010 — Room: 213 — Location: Washington State Convention Center

Session Chairs: Christopher Schuh, MIT; John Lewandowski, Case Western Reserve University

2:00 PM Invited
Influence of Condensed Bond Enthalpy on Metallic Glass Stability: *Dan Miracle*[1]; Garth Wilks[2]; Amanda Dahlman[3]; [1]AF Research Laboratory; [2]General Dynamics, Inc.; [3]SOCHE

While empirical guidelines suggest that the enthalpy of mixing influences glass stability, previous work has failed to show a correlation. This work seeks to establish a connection between nearest neighbor bond energy and glass-forming ability through evaluation of interatomic bond enthalpies. An approach to determine bond enthalpies from available thermodynamic data will be briefly described and resulting bond enthalpies will be presented. The number and type of atom bonds that are present in a metallic glass structure are estimated as a function of metallic glass constitution using the efficient cluster packing structural model. By combining these two analyses, we estimate the enthalpy associated with glass formation, and explore correlations with experimental measurements of glass-forming ability.

2:20 PM
Model Experiments to Mimic Fracture Surface Features in Metallic Glasses: *Lisa Deibler*[1]; John Lewandowski[1]; [1]Case Western Reserve University

The purpose of this study is to examine how changes in viscosity, specimen geometry, and degree and type of inhomogeneity affect the fracture surface observations on a model of metallic glass fracture. Experiments were conducted on tensile samples of various geometries constructed to contain liquids of different viscosity that were tested at three temperatures. The influence of mixtures, layers, and dispersions of two different viscosity materials on the fracture surface features was also investigated. The observed fracture surfaces of these viscous materials were quantitatively examined to provide a comparison with surface features found in several metallic glasses.

2:30 PM Invited
Modeling the Mechanical Behavior of Metallic Glasses Using STZ Dynamics: Eric Homer[1]; *Christopher Schuh*[1]; [1]MIT

Recent advancements in a meso-scale model for the mechanical behavior of metallic glasses have allowed a single modeling technique to bridge the disparate timescales associated with different modes of deformation in a metallic glass, a task which has proven difficult using other modeling approaches. A discussion of the modeling technique, which is based on the shear transformation zone, and its application using finite element analysis and the Kinetic Monte Carlo algorithm are presented. Recent analyses of simulations performed with this technique elucidate the conditions under which spatial and temporal correlations between shear transformation zones lead to different modes of observed macroscopic deformation. These correlation analyses provide some of the first insights into the localized microscopic processes that lead to inhomogeneous deformation analogous to nascent shear banding. Details regarding the extension of the modeling technique to three-dimensional systems and complex loading conditions are discussed.

2:50 PM
Continuum Model for Bulk Metallic Glass Composites: *Fadi Abdeljawad*[1]; Mikko Haataja[1]; [1]Princeton University

Recent experimental work has suggested that the problem of catastrophic failure by shear band propagation in Bulk Metallic Glasses (BMGs) can be solved by forming composites with a two-phase microstructure consisting of the glassy BMG matrix phase and a non-percolating, soft crystalline phase. In this talk, we present a continuum model of plastic deformation in two-dimensional BMG composites. The elastic energy density is a periodic nonlinear function of the strains, while the structural heterogeneity of the glassy phase is accounted for by defining a quenched, spatially varying random variable that corresponds to the maximum local strain needed to cause a slip event. Simulations of BMGs with various sizes of crystalline domains under simple shear loading show that deformation patterns and mechanical strength are affected by the area fraction and spatial distribution of the crystalline domains, implying a size effect in the strength of BMG composites.

3:00 PM Invited
Deformation and Failure of Glasses at Nanoscale: *Ju Li*[1]; Erik Bitzek[1]; [1]University of Pennsylvania

Recent experiments on nanoscale amorphous materials have suggested interesting ductility - size scale dependencies (PNAS 104, 11155; PRB 77, 155419). Such size effect may shed light on the connection between plastic deformation and underlying spatio-temporal hierarchies of structural flow defects, the smallest of which is a single shear transformation zone (STZ) ~1nm^3. A mesoscale computational model (on the same level as discrete dislocation dynamics for crystalline materials) is constructed, which utilizes detailed statistical information about shear transformations, damage accumulations and damage repairs from atomistic simulations. Adjacency to surfaces/interfaces and the loading constraints could have strong effect on the apparent ductility of nanoscale glasses.

3:20 PM
Numerical Deformation Simulations on Bulk Metallic Glasses Using First-Principles Methods: *Lizhi Ouyang*[1]; Despina Louca[2]; Gongyao Wang[3]; Yoshihito Yokoyama[4]; Peter Liaw[3]; [1]Tennessee State University; [2]University of Virginia; [3]University of Tennessee; [4]Tohoku University

It was found recently that the cyclic fatigue loading causes the local structure changes in Zr-Cu-Al bulk metallic glasses (BMG). To reveal their atomistic origins, we performed numerical fatigue tests on Zr50Cu40Al10 and Zr60Cu30Al10 (in atomic percent) using first-principles methods. Large periodic models with 600 atoms are constructed for the two metallic glasses using the quenching and annealing technique. The local strain distributions of the deformed models generated by the numerical fatigue loadings are analyzed to identify irreversible structural changes and potential shear-band nucleation sites. The structure evolutions of the two BMGs under numerical cyclic loading are examined and the changes in their pair distribution functions are compared with the experimental results.

3:30 PM Break

3:40 PM Invited
Simulating Poisson Ratio Effects on Shear Banding Behavior in Metallic Glasses: *James Morris*[1]; Takeshi Egami[2]; [1]Oak Ridge National Laboratory; [2]University of Tennessee

Shear banding occurs commonly during deformation of bulk metallic glasses, often leading to failure. Understanding and controlling this phenomenon is important to improving the properties of metallic glasses. Several studies have suggested that an increased Poisson ratio is correlated with improved mechanical properties; for example, the fracture energy can change by three orders of magnitude as the Poisson ratio changes from 0.3 to 0.4 [J. J. Lewandowski et al., Phil. Mag. Letters 85, 77-87 (2005)]. To understand this behavior, we have begun molecular dynamic simulations of glasses under simple shear, using a model with a tunable Poisson ratio. The inhomogeneous shearing behavior is examined as a function of Poisson ratio, temperature, and strain rate. These results are compared with a phenomenological model which predicts the coexistence of two states with distinct viscosities.

This research was sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy.

4:00 PM
Reverse Monte Carlo Simulation of Medium-Range Atomic Order in Bulk Metallic Glass Incorporating Fluctuation Electron Microscopy: *Jinwoo Hwang*[1]; Paul Voyles[1]; [1]University of Wisconsin Madison

We have investigated medium-range order in Zr-based BMGs using fluctuation electron microscopy (FEM) and Reverse Monte Carlo (RMC) simulation. Initial RMC simulations incorporating FEM and electron diffraction reduced density function (RDF) data showed that including FEM data in RMC more uniquely confines the short to medium-range atomic structure compared to RDF data alone, and that the FEM signal is likely to arise from nanometer-scale planar order in the structure. However, the MRO in the model was anisotropic due to limitations in the simulation and experiment. Improved FEM data obtained using highly-coherent, variable probe-size nanodiffraction in an aberration-corrected STEM will be presented, as will the results of more isotropic FEM RMC simulations which incorporate approximate chemical information in the form of EAM empirical potentials.

4:10 PM
Reliability of Methods of Computer Simulation of Structure of Amorphous Alloys: *Mikhail Mendelev*[1]; Mattew Kramer[1]; [1]Ames Laboratory

There are several computer simulation methods to generate atomic models of glasses. We analyzed advantages and disadvantages of these methods. We took a model created by the MD simulation with a semi-empirical potential as a target system and explored how its structure can be reproduced using different simulation techniques. First, we explored effect of the cooling rate and found that if the cooling rate is ~ 10^13 K/s the system has no time to adjust its structure to the change in temperature/density. It was also found that a small model size used in ab initio MD simulations can affect the final structure. Finally we used the target PPCFs to explore a possibility to create the atomic models from diffraction data using the RMC method. We created models with the PPCFs which almost coincided with the target ones but the structure of these models was different from the target structure.

4:20 PM Invited
Connecting Atomic Structure and Plastic Deformation in Zr-Based Bulk Metallic Glasses: *Paul Voyles*[1]; Jinwoo Hwang[1]; Jonathan Puthoff[1]; Don Stone[1]; [1]University of Wisconsin, Madison

We have recently used broadband nanoindentation creep to measure the volume of shear transformation zones (STZs) in three Zr-Cu-Al alloys in the context of the Johnson-Samwer cooperative shear model of plastic deformation. The STZs occupy 100-300 atomic volumes, which corresponds to spheres 1.5 to 2 nm in diameter. We use fluctuation electron microscopy (FEM) to measure structure at this length scale, which is difficult to access from more conventional techniques. Reverse Monte Carlo simulations incorporating FEM data show that consistency with FEM requires nanoscale regions with pseudo-planar order in the model and constrains the partial pair distribution functions. Higher-quality, variable probe-size FEM data from a new aberration-corrected STEM and hybrid reverse Monte Carlo simulations incorporating EAM potentials for Zr-Cu-Al will be presented.

4:40 PM
Computational Studies on Free Volume and Plastic Flow in Metallic Glasses: *Joshua Askin*[1]; Ashwini Bharathula[1]; Wolfgang Windl[1]; Katharine Flores[1]; [1]The Ohio State University

Positron annihilation spectroscopy studies reveal a trimodal lifetime distribution corresponding to 3 distinct defect volume ranges in bulk metallic glass structures which evolve in a regular manner with plastic deformation. These volumetrically distinct defects are hypothesized to be inherent interstitial holes, flow defects and nano-scale voids. To test this hypothesis, we developed an electron density model based on radial averaging of ab-initio charge density,[1] which we use to visualize evolution of "free/excess" volume or lower density regions during MD annealing and deformation. Rather than using different cooling rates to control density, a series of voids are injected into the glass structure under constant volume conditions. Under constant-volume annealing, the void redistributes amongst other defects. Under constant-volume shear, strain localization only occurs above a critical void size, indicating a requisite combination of applied shear and available excess volume. References[1] Metallurgical and Materials Transactions A, 39A 2008 1779-1785.

4:50 PM
Structure and Anelastic Relaxation in Metallic Glasses: *Garth Wilks*[1]; Daniel Miracle[1]; Amanda Dahlman[1]; [1]Air Force Research Laboratory

Variation in the constitution of several metallic glass ribbons are used to probe their deformation activation energy spectra via anelastic bend stress relaxation. The specific effects of vacancy and anti-site defects predicted by the Efficient Cluster Packing model are used to rationalize deviations in spectra between material conditions, particularly the effects that the energy, type, and concentration of such defects contribute to local free volume dilatation and their ability to act as sites for unit shear process nucleation.

5:00 PM
Avalanches, Size-Effects, and Critical Behavior in Shared Model Metallic Glasses: K. Michael Salerno[1]; *Craig Maloney*[2]; Mark Robbins[1]; [1]Johns Hopkins; [2]Carnegie Mellon University / Civil & Environmental Engineering

We perform computer simulations of sheared binary Lennard-Jones glasses in 2D at zero temperature and in the limit of small strain rate. The strain energy is released in discrete bursts with a Gutenberg-Richter size distribution. The plastic strain is organized into lines of slip which accumulate during avalanches over a system-size dependent characteristic strain scale deltagamma_c. deltagamma_c should give rise to interplay between indentation rate and system size which may be observable in micro-pillar indentation experiments on metallic glasses. Furthermore, we show that the spatial organization of the plastic deformation has a novel kind of fractal geometry, with orientation-dependent scaling exponents. These results further suggest that micro-pillar indentation experiments performed on bulk-metallic glass samples should exhibit a kind of self-organized critical behavior similar to that observed in crystalline samples [1]. [1] Dimiduk, DM , et al. Science 312 (5777). 1188-1190 (2006).

5:10 PM Invited
Stress and Temperature Induced Phase Transformation in Zr-Based Metallic Glass via Molecular Dynamics Simulation: *Yunche Wang*[1]; Chun-Yi Wu[1]; Jinn Chu[2]; Yanfei Gao[3]; Peter Liaw[3]; [1]National Cheng Kung University; [2]National Taiwan University of Science and Technology; [3]The University of Tennessee

Transformation between crystalline and amorphous phases in the Zr47Cu31Al13Ni9 metallic glass is studied with the molecular dynamics (MD) simulation to understand atomic stress and strain distributions under uniaxial stress and various heat treatments. In this paper, a molecular model of the Zr-based metallic glass is obtained by sputter MD simulation. Then, a portion of the as-deposited film is used as initial structures for uniaxial tension/compression tests and heat treatment. The discontinuity in volume change upon heating is observed around the Tg of the metallic glass, and corresponding microstructures are studied. It is found that the uniaxial compression of the glass has superior plasticity than that of its tensile behavior. Atomic stress and strain calculations reveal atomic constitutive relationships to facilitate identification of microstructural changes.

5:30 PM
Directional Deformation Memory and Orthogonal Bauschinger Effect in Metallic Glasses: *Erik Bitzek*[1]; David Rodney[2]; Ju Li[1]; [1]University of Pennsylvania; [2]Institut Polytechnique de Grenoble

In crystalline materials the Bauschinger effect whereby plastic deformation in one direction leads to a different deformation behavior upon re-straining in the opposite direction is well known. In bulk metallic glasses (BMGs) however, no such effect has been reported. Furthermore, as the free-volume model of plastic deformation is inherently isotropic, the accumulation of damage is usually believed to be directionally independent, as long as no shear bands are formed. Here we present results of MD simulations on BMGs which show a directional dependence of the deformation memory: when strained along one axis and then unloaded, the samples show a different deformation behavior depending on whether they are strained again in the same direction, or orthogonal to the initial loading direction. The simulations are compared with recent experiments, and the origin of the orthogonal Bauschinger effect is discussed in terms of the directional properties of the shear transformation zones.

5:40 PM
Atomistic Simulations to Estimate Plasticity of Cu-Zr Bulk Metallic Glasses: *Kyung-Han Kang*[1]; Byeong-Joo Lee[1]; [1]POSTECH

Understanding the origin of and thus improving the plasticity is one of the hot issues in the bulk metallic glass (BMG) society. Many reports suggest that plasticity of BMGs may be correlated with several properties such as free volume, short range ordered structure, the ratio of shear modulus to bulk modulus, Poisson's ratio, atomic displacement and viscosity. In this study, a special attention was focused on the evaluation of the correlation between the above mentioned properties and plasticity in the Cu-Zr binary BMGs, by comparing the experimentally reported composition dependence with that of various properties obtained from atomistic calculations based on a modified embedded-atom method (MEAM) interatomic potential. It was found that the free volume and the distribution of short range ordered structures have a relatively clear correlation with plasticity. The correlation between the plasticity and other individual properties will also be presented.

Carbon Management and Carbon Dioxide Reduction: Session I

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS Extraction and Processing Division, TMS: Energy Committee
Program Organizers: Subodh Das, Phinix LLC; Brajendra Mishra, Colorado School of Mines; Neale Neelameggham, US Magnesium LLC

Wednesday PM — Room: 310
February 17, 2010 — Location: Washington State Convention Center

Session Chair: Subodh Das, Phinix , LLC

2:00 PM
Upcoming Carbon Management Legislations: Impacts and Opportunities for the Global Aluminum Industry: *Adam Gesing*[1]; Subodh Das[1]; [1]Phinix, LLC

The European Union is planning to include the aluminum industry in its carbon management system in 2013. Additionally, if and when enacted, "The American Clean Energy and Security Act" of 2009 will also force U.S. industries to comply with much debated "carbon cap and trade" system. The Waxman and Markey legislation – along with the Environmental Protection Agency mandate under the Clean Air Act – will specifically include US aluminum industry with CO2 equivalent sources of more than 25,000 tons per year. This paper will review the carbon management system as it now operates and how it is likely to be applied to the European and American aluminium industry.

2:30 PM
Cost-Effective Gas Stream Component Analysis Techniques and Strategies for Carbon Capture Systems from Oxy-Fuel Combustion (An Overview): *John Clark*[1]; Danylo Oryshchyn[1]; Thomas Ochs[1]; Steve Gerdemann[1]; Cathy Summers[1]; [1]National Energy Technology Lab

Limited analysis of combustion gas streams where carbon capture is not of interest is done mainly to ascertain operation parameters. Stringent regulations on acid gases and particulates promote careful flue gas analysis. Unregulated components are typically not analyzed.Typically not more than four points (two in the boiler and one each in the flue and the stack) are sampled. A successful oxy-fuel process with carbon capture and compression is anticipated to require a many as 12 sample points with analysis for water, nitrogen, oxygen, argon, NOx, SOx, and carbon monoxide. Carbon dioxide captured for beverages produces a high value product and the cost associated with analysis is warranted. However, carbon capture for disposal must keep all costs to a minimum. This paper will compare alternative approaches for cost-effective sampling and analysis of the carbon dioxide product streams from oxy-fuel combustion, through all stages of production through compression and pipeline/vessel delivery.

3:00 PM
Strategic Approaches for CO2 Reduction Rate from Fossil Fuel Use in Steel Industry: *Malti Goel*[1]; [1]INSA

Technology advancements in fossil fuel based energy generation are currently being aimed at minimization of CO2 emissions. To attain energy security, India must accelerate the pace of economic development, while achieving reduction in CO2 emissions per unit of energy. It would need access to advanced coal utilization technologies to be demonstrated on indigenous coal characteristics. Of specific importance would be: improvement in coal quality, increasing efficiency of fossil fuel use, and suitability of other CO2 sequestration technologies for reducing CO2 footprints. There is need to address related risks and financial burden through adoption of policies and regulations including the issue of open access in energy research. In this paper, seven important areas of strategic plan that need to be pursued for managing CO2 emissions in energy sector are discussed. A case study from steel industry is presented.

3:30 PM
Development of Reverberatory Furnace Using in Copper Scrape Smelting by Reformed Natural Gas: *Mohamed Ahmed Hammad*[1]; [1]CMRDI

Reverberatory furnace which used for smelting of scrape of copper, residual anodes and cathodes from the next stages which carried out in copper after casting from this furnace using wood as a resource of reduction gases such carbon monoxide, hydrogen and methane. That is the problem, using of wood causes the following: (1) Pollution of medium of copper melting (forming soot of smock above furnace) (2) low efficiency in removal of oxygen from copper and more contamination in copper matte causes in rising of heat to remove of it and increasing in cost and time of casing of copper (3) high expensive this problem was solved by using of reformed natural gas as a source of reduction gases (CO+ H2).

4:00 PM Break

4:15 PM
Bauxite Residue Neutralization with Carbon Sequestration: *Luis Venancio*[1]; Emanuel Macedo[2]; Antonio Ernandes Paiva[1]; José Antonio Souza[2]; [1]Federal Institute of Education Science and Technology - Maranháo; [2]Universidade Federal do Pará

The production of alumina from bauxite using the Bayer process generate 1.25 ton of the residue known by red mud and 460 kg of CO2 per ton of alumina. The direct use of exhaust gases from the alumina refineries to react and neutralize the bauxite residue may allow a double gain: open a wide range of new applications for bauxite residue reducing the reactivity of red mud and sequester approximately 15% or 67 kg of CO2 per ton of alumina.This paper shows the reaction of a suspension of bauxite residue-water with a simulation of the calcinator exhaust gases of the refinery. The influence of the temperature and the ratio water red mud is also analyzed.

4:45 PM
Electrochemical Quartz Crystal Microbalance Study on Carbon Dioxide Adsorption in the Presence of Electrosorbed Hydrogen on Cu-Gold Single Crystals: *Maria Salazar-Villalpando*[1]; [1]National Energy Technology Laboratory

Finding areas of CO2 utilization represents an opportunity to decrease global warming. The electrochemical reduction of CO2 could represent a form of energy storage. Tests of carbon dioxide adsorption on Cu-Gold single crystals are a preliminary step in the study of CO2 electrochemical conversion. The electrochemical deposition of Copper is studied with the electrochemical quartz crystal microbalance (EQCM) on a gold substrate. Cu is deposited from acidic sulphate bath. Cyclic voltammograms are obtained to determine electrical potentials for copper deposition on Au-single crystals. Moreover, electrical potentials for products generated between electrosorbed Hydrogen and CO2 molecules are investigated.

5:10 PM
The Thermal Gas Processing in Pre-Heating Zone of "Water-Jacket" Furnaces in "Trepça": *Ahmet Haxhiaj*[1]; Egzon Haxhiaj[2]; [1]University of Prishtina; [2]American University in Kosovo

The paper has as a studying object the issue of effective management of gasses' heating and dusts in reducing melting process in lead (Pb) metallurgy. It also analyses the issue related to the usage and recycling of dusts and gasses in all pyro-metallurgical processes of technical lead production. The paper contains the analysis of technological process of separation of humidity, gasses, and dusts of valuable remainders in "Trepça" plant. Paper has the results of theoretical-experimental studying, analytical and graphical of gasses thermal balance depending on height and composition of load, and the coke quantity on load for reducing melt in "Water-Jacket" furnaces. With thermal balance, having into consideration all parameters of heat in entry and exit depending on aforementioned factors we aimed to optimize the parameters of the process, keeping the attention to the minimization of energy consumption, and the overall influence on environment.

5:35 PM
Oxidation Kinetics of Fe-Cr and Fe-V Liquid Alloys under Controlled Oxygen Pressures: *Haijuan Wang*[1]; Nurni Viswanathan[2]; Seshadri Seetharaman[1]; [1]Royal Institute of Technology(KTH), Sweden; [2]Indian Institute of Technology Bombay, Mumbai,India

The oxidation kinetics of Fe-Cr as well as Fe-V alloys were investigated with CO2 as the oxidant gas by thermogravimetric analysis (TGA) in the temperature range 1550-1650°. Further, the gas-liquid reaction sequence was monitored by X-ray radiographic observations at 1600°. The results of the TGA experiments show clearly that the oxidation proceeds at a slower rate when pure CO2 is used as the oxidizer compared with different CO2-O2 mixtures. The post-measurements samples were subjected to chemical analysis, SEM-EDS and XRD analysis. The result indicated that the oxide scale was mainly a spinel phase; the oxidation of iron was found to occur alongside the oxidation of chromium and vanadium. The oxidation was taking place in steps indicated by the changes in the slopes of the thermogram for oxidation as a function of time. In general, rates of oxidation decrease after achieving a maximum value through an initial transient.

Cast Shop for Aluminum Production: Cast House Productivity and Strip Casting

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee, TMS: Aluminum Processing Committee
Program Organizers: John Grandfield, Grandfield Technology Pty Ltd; Pierre Le Brun, Alcan Voreppe Research Center

Wednesday PM Room: 609
February 17, 2010 Location: Washington State Convention Center

Session Chair: Philippe JARRY, Unité de Recherches Fonderie ALCAN CRV

2:00 PM
Means of Improving Casthouse Productivity: *Peter Whiteley*[1]; [1]Munimula Technology Pty Ltd

This presentation will deal with ways of improving casthouse productivity by commencing with management issues concerned about product mix, organisation, potroom interface in a smelter context and the fabrication interface in a remelt context, production and maintenance planning, training and culture. Following this introduction, the next matters to be considered are means to maximise asset utilisation by examining a suite of opportunities including process intensivity, debottlenecking, benchmarking, scrap reduction, data logging, trending and use of algorithms, compiling multiple activity charts, identification of root causes of delays and aborts, conducting dynamic simulations, adaption of new technologies, melt loss minimisation, and other ways of improving plant OEE. The presentation will cover smelter based casthouses as well as remelters and scrap based operations, since each have specific challenges and opportunities.

2:25 PM
Estimating the Production Capabilities of Casthouse Equipment Configuration Options: *Phillip Baker*[1]; [1]Hatch Associates

Operational Casthouses must, above all else, be capable of accepting all primary metal produced by the Potlines so as not to limit the ability of the smelter to produce metal and to provide the most stable operating regime for the reduction cells by allowing consistent metal pad depth. To be effective, Casthouse equipment configurations must accommodate not only the Normal operational state, but also both Repair and Catch-Up scenarios. Hatch has developed a simple first pass methodology for assessing the performance of equipment configuration options for primary aluminium Casthouses in this context.

2:50 PM
Electrochemical Characterization of TRC 7072AA for Heat Exchangers: *Aziz Dursun*[1]; Beril Corlu[1]; Canan Inel[1]; Murat Dundar[1]; Rasim Erdogan[1]; Mustafa Ürgen[2]; [1]Assan Aluminium; [2]Istanbul Teknik Üniversitesi

We present the results of corrosion potential measurments of DC and TRC cast 7072AA used as a fin material in mechanical heat exchanger applications. The alloys used were continuously cast to two different gauges and Zn,Ti Fe and

Si content, using twin roll casting technology. Optic and electron microscopy with x-ray EDS capability was used to corrolate the electrochemical results with microstructure and chemical composition at the surface. It was shown that higher solidification rates developed during twin roll casting at much thinner gauges resulted in much lower corrosion potentials. This in turn made us possible to reduce Zn content to improve the thermal conductivity while maintaining the desired corrosion potential. Unlike Zn and Ti, higher concentrations of Fe and Si added with the purpose of retaining adequate strength at much thinner thicknesses do not have an adverse effect on corrosion potentials.

3:15 PM

Influence of the Cooling Water Temperature on Productivity and Product Quality in Twin Roll Casting with Copper Shells: *Mark Badowski*[1]; Eduardo Garate[1]; David Armendariz[1]; [1]Hydro Aluminium

The use of twin roll casters for the production of aluminium strip is today widespread. The twin roll casting process offers advantages such as reduced investment and energy costs or a fine grained microstructure. However, the production volume compared to the DC-casting process is limited by the low productivity and restricted alloy range. Utilization of copper shells can increase productivity through improved heat extraction at the solidification interface. Increased heat flux can impact several other parameter like strip profile and mechanical properties. A better understanding of this complex relationship is required to fully utilize the potential of this new technology.The present paper describes operational experiences at Hydro Aluminium INASA obtained with copper shell technology. The productivity and product quality achieved after implementation is compared to previous numerical predictions. The influence of the cooling water temperature is discussed including the productivity and product quality achieved through optimization work.

3:40 PM

The Use of Copper Shells by Twin Roll Strip Casters: Aldenir Clemente[1]; John Tsiros[2]; Aristeidis Arvanitis[2]; *Dionisis Spathis*[2]; Hans-Gunter Wobker[3]; [1]Castcom Ltda; [2]Hellenic Aluminium Industry SA (Elval SA); [3]KME Europe

Twin roll casting of aluminum alloys is a well established process, which exists over several decades. The productivity of the process has been largely limited by the heat transfer capability of the steel shells used on the caster rolls. In recent years, developments in the manufacture of shells based on special copper alloys have opened a window for productivity increases and quality improvement. One or both rolls of a caster can be lined with copper shells, to take advantage of the higher thermal conductivity of Cu relative to Fe, which provides for an increased cooling capacity of working rolls.This paper presents a review of the equipment/operation, productivity increase and product/quality performance, by using both copper/copper and copper/steel combination

4:05 PM

A TEM Study of the Microstructures of 3003 and 3003-Zr Alloys Produced by Twin Roll Casting: *Beril Corlu*[1]; Ozgur Duygulu[2]; Selda Ucuncuoglu[2]; Gizem Oktay[2]; Aziz Dursun[1]; Murat Dundar[1]; [1]Assan Aluminum; [2]TUBITAK MAM

3003 is a typical alloy produced with twin roll casting (TRC)technology for various application of industry. Alloying of 3003 with Zr has been studied for conventional production technique, i.e. DC casting and hot-rolling. However, it has not been investigated for a similar composition solidified at the cooling rate of TRC. In this study, the microstructures of TRC 3003 and ~0.08 wt.% Zr containing TRC 3003 alloys were investigated using optical microscopy (OM), scanning electon microscopy (SEM) and transmission electron microscopy (TEM). For both alloys, the same thermomechanical downstream process was employed, which included a homogenization treatment at an intermediate thickness and a final annealing. Intermetallic particle evolution after the annealing steps was investigated comparatively. Recrystallization temperature of TRC 3003 alloys were significantly altered with the addition of ~0.08 wt.% Zr due to the formation of Zr containing second phase particles.

4:30 PM

Casthouse Design for the Production of Air-Cooled, Low-Profile Aluminium Sows: *Tom Plikas*[1]; Tony Cesta[1]; Lowy Gunnewiek[1]; Michael Trovant[1]; Rui Santiago[1]; Jean Vanasse[2]; [1]Hatch Ltd.; [2]Aluminerie Alouette Inc.

The Aluminerie Alouette Inc. Smelter in northern Quebec, Canada recently completed a major plant expansion that includes a new casthouse for the continuous production of low-profile aluminium sows using natural air cooling technology. This is a novel concept representing a departure from the traditional batch, water-cooled casting operations of the past, and has benefits in terms of sow quality, production efficiency, safety, and mould maintenance. The casthouse design presented many challenges: ensuring proper casting and cooling of sows at the correct metal production rate to produce high quality sows, design of the casting machine and moulds to withstand thermal shocks and stresses, developing a ventilation system for effective management of heat released during the casting process, and protection of heat sensitive equipment and instrumentation using radiation shielding. This paper describes how these engineering challenges were met through the use of sound design practice, empirical testing, and computational methods.

4:55 PM

The Measurement of Heat Flow within a DC Casting Mould: *Arvind Prasad*[1]; John Taylor[1]; Ian Bainbridge[1]; [1]University of Queensland

The heat flow between the molten metal and the mould-wall in DC casting is often assumed to be negligible compared to that due to the sub-mould water cooling. Furthermore, the entire DC casting process is often described based on this assumption. However the assumption of negligible heat transfer in the metal-mould region and its subsequent minimal influence on cast product quality remains unproven. The focus of the present paper is therefore on understanding the heat transfer in the metal/mould wall region. To this end a method for the laboratory measurement of the flow of heat from the metal being cast to the wall of a DC casting mould has been developed. The equipment and methodology are briefly described together with the initial results obtained. The implications of this work for use in simulation models and for the design and operation of DC casting moulds are discussed.

Characterization of Minerals, Metals and Materials: Characterization of Cu, Zn, Mn, Fe, Au, and Carbon Phases

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division, TMS Structural Materials Division, TMS/ASM: Composite Materials Committee, TMS: Materials Characterization Committee

Program Organizers: Ann Hagni, Geoscience Consultant; Sergio Monteiro, State University of the Northern Rio de Janeiro - UENF; Jiann-Yang Hwang, Michigan Technological University

Wednesday PM — Room: 307
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Tzong Chen, CANMET-MMSL; Yoshitaro Nose, Kyoto University

2:00 PM Introductory Comments

2:10 PM

Ternary Phase Diagram of the Zn-Sn-P System for Fabrication of $Znsnp_2$ Compound Semiconductor: *Yoshitaro Nose*[1]; Noriyuki Tanaka[1]; Tetsuya Uda[1]; [1]Kyoto University

Recently, solar cells using compound semiconductors such as $Cu(In,Ga)Se_2$ with chalcopyrite structure attract much attention. However, the compounds consist of In and Ga, which are rare elements, and Se with toxicity. We thus focus on $ZnSnP_2$, which has also chalcopyrite structure and consists from safe and abundant elements. Additionally, its bandgap varies from 1.66 eV to 1.25 eV. In this study, we try to fabricate $ZnSnP_2$ based on ternary phase diagram of the Zn-Sn-P system. First, we establish the phase diagram by equilibrium experiments using zinc, tin and their phosphides. At 700 ºC, $ZnSnP_2$ is almost stoichiometry, while its single-phase region ranges to Zn-rich composition at 600 ºC. It is also obtained that $ZnSnP_2$ is stable at higher temperatures than literature data. Some differences with the previously reported diagram of the $Sn-ZnP_2$ pseudo-binary system have been clarified and the diagram of the system has been re-constructed.

2:35 PM
Microstructure Evolution in Copper-Clad-Steel and Copper-Clad-Aluminum Bimetallic Wires during Drawing Processes: *Taisuke Sasaki*[1]; Robert Morris[1]; Karen Torres[1]; Gregory Thompson[1]; Y. Syarif[2]; D. Fox[2]; [1]University of Alabama; [2]Fushi Copperweld, Inc.

Bimetallic wires combine the features of dissimilar metals to achieve a cost and/or a performance advantage over solid metal conductors in applications such as battery cables, coaxial cables, and grounding. In high frequency applications, the copper-clad steel provides a high strength alternative and the copper-clad aluminum offers a low weight option. The thermomechanical and microstructure evaluation in these simultaneously co-deformed materials are compared at different drawing stages. In the as-drawn condition, a filamentary granular microstructure forms along the closest packed directions as quantified by SEM-EBSD. The copper sheath also shows deformation twins. The cold worked drawing passes have a corresponding increase in hardness as a function of reduced area per pass. The hardness is lowered with a loss of preferred texture during intermediate heat treatments because of recrystallization. Nanoindentation hardness of the drawn wires has been measured across the bimetallic interfaces and compared to TEM-EDX compositional profiles.

3:00 PM
OIM Characterization of a Jewelry Gold Alloy Subjected to Small-Charge Explosion: Chiara Pozzi[1]; John Bingert[2]; *Donato Firrao*[1]; [1]Politecnico di Torino; [2]Los Alamos National Laboratory

As part of a wider experimental campaign a gold alloy sample was exposed to a blast from 100 g of plastic explosive, at a charge-to-sample distance of 220 mm. From optical microscopy observations, the occurrence of very fine deformation features on the surface exposed to the blast wave was documented. Due to the high deformation rate related to an explosive-generated shock, the occurrence of deformation twinning was suspected. Orientation imaging microscopy was employed to investigate the actual nature of the deformation marks observed by optical microscopy. Results obtained on the post-mortem sample are presented and compared to those of the as-prepared condition.

3:25 PM
Characterization of Tin-Rich Copper Anodes from Secondary Copper Refineries: *Tzong Chen*[1]; John Dutrizac[1]; [1]CANMET-MMSL

Copper anodes generated from copper scrap are relatively rich in Sn, Zn and Fe. Because of the presence of oxygen, only trace amounts of Sn are present in solid solution in the copper crystals. Thus, Sn occurs mainly as SnO2, Cu-Sn-Ni oxide and Sn-Ni-Zn oxide in the copper anodes, and Zn and Fe occur mainly as minor constituents in the Sn-Ni-Zn oxide and Cu-Sn-Ni oxide. During electrorefining, these oxide species are liberated directly from the copper anodes and report to the anode slimes. The trace amounts of Sn, present in solid solution in the copper crystals, dissolve but reprecipitate as Sn arsenate or a Sb-As-Sn-O phase. Accordingly, high Sn contents in copper anodes do not lead to elevated Sn concentrations in the electrolyte.

3:50 PM
Study on the Interface Behavior of Ore Powder in the Organic Media: *Li Dan*[1]; Chen Qiyuan[1]; [1]Central South University

In this paper, pyrite ore powder for the raw materials, acetone, chloroform, cyclohexane, cyclohexanol, toluene, tetrahydrofuran, sodium dodecyl sulfate to organic solvents, n-dodecanethiol as a modifier, study from the dispersion of yellow iron ore body in this organic solvent interface in seven acts. Dispersion in the study, with photographs of law, ultraviolet spectroscopy, oscillation, scanning electron microscopy, and electron spin resonance method in the seven types of pyrite in the organic solvent dispersion of research. The experimental results for the pyrite in sodium dodecyl sulfate in the dispersion of the best, followed by tetrahydrofuran, followed by cyclohexanol, chloroform dispersion of the worst. After pyrite modified with ESR analysis showed that iron ore yellow surface a series of localized paramagnetic state. Samples of the modified scanning electron microscope results show that modified after treatment in n-dodecanethiol smaller lattice.

4:15 PM
Synthesis of ZnO/TiO2 and Study on its Photocatalytic Activity: *Wu Daoxin*[1]; [1]Changsha University of Science and Technology

With $Ti(C_4H_9O)_4$ and $Zn(Ac)_2{\bullet}2H_2O$ used as raw materials, oxalic acid as the complexing agent and anhydrous ethanol as solvent. the ZnO/TiO_2 photocatalytic nanocomposite materials was prepared by Sol-gel method and characterized by XRD,DRS and FS, and catalyst for photodegradation experiments. The results show that when TiO_2 composite is 40% (mole fraction), calcination temperature is 400°,ZnO/TiO_2 has a good absorption performance, which indicated that red shift occurred. With sunlight as the light source, pH=5.0, catalyst concentration is 1.0mg.L^{-1}, concentration of methyl orange is 5.0mg.L^{-1}.The result shows that ZnO/TiO_2 powders(40%,400°) has the most photodegradation efficiency, and the degradation efficiency of 96.5% after 4 hours.

4:40 PM Concluding Comments

4:50 PM Question and Answer Period

Cost-Affordable Titanium III: Creative Processing and Property Enhancement II

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS: Titanium Committee
Program Organizers: M. Ashraf Imam, Naval Research Lab; F. H. (Sam) Froes, University of Idaho; Kevin Dring, Norsk Titanium

Wednesday PM   Room: 618
February 17, 2010   Location: Washington State Convention Center

Session Chairs: Mitsuo Niinomi, Toyohashi University of Technology; Rodney Boyer, Boeing Commercial Airplanes

2:00 PM
Rapid Consolidation of Ti-6Al-4V Powders by Transformation Superplasticity: Bing Ye[1]; Marc Matsen[2]; *David Dunand*[1]; [1]Northwestern University; [2]The Boeing Company

The densification kinetics of Ti-6Al-4V powders with spherical or angular shapes are compared in uniaxial die pressing experiments between isothermal conditions (at 1020 °C, in the beta-field, where deformation occurs by creep) and during thermal cycling (860-1020 °C, within the range of the alpha-beta phase transformation of the alloy, where transformation-mismatch superplasticity is activated). Densification kinetics are markedly faster under thermal cycling than under isothermal conditions, as expected from the higher deformation rate achieved under transformation-mismatch plasticity conditions as compared to creep conditions. The densification curves are successfully modeled for both creep and superplastic deformation mechanisms using (i) simple closed-form solutions and (ii) the finite-element method. Densification kinetics, under isothermal and thermal cycling conditions, of Ti-6Al-4V powders containing 5-20 vol.% ceramic particles are also presented.

2:25 PM
Evaluation of Titanium for Vehicle Fuel Economy and Performance Improvement: P.K. Mallik[1]; *Curt Lavender*[2]; Scott Weil[2]; [1]University of Michigan at Dearborn; [2]Battelle - Pacific Northwest National Laboratory

The potential for titanium to decrease the mass of propulsions system in a vehicle have been studied and used to predict the increase in fuel efficiency of a vehicle. The overall efficiency improvement will come not only from titanium substitution but also from downsizing or material substitution of other interacting components resulting in reduced engine friction losses and inertia force reduction in reciprocating and rotating components. Candidate components for titanium have been identified and low cost processing routes have been identified for each component using emerging low cost titanium raw materials and processing routes.

2:50 PM
Titanium Recycling Process by Disproportionation of Titanium Subchloride in Molten Magnesium Chloride: *Taiji Oi*[1]; Toru Okabe[1]; [1]The University of Tokyo

In order to establish a new titanium recycling process, the synthesis of TiCl2 from Ti scrap heavily contaminated with Fe and the production of pure Ti by the disproportionation of TiCl2 in molten MgCl2 were investigated. TiCl2 containing small amount of Fe was synthesized by reacting TiCl4 with heavily contaminated Ti scrap (Ti-44%Fe-9%Cr-5%Ni) in by utilizing MgCl2 molten salt as a reaction medium at 1273 K. Ti powder with a purity of over 99% was obtained by the disproportionation of TiCl2 in molten MgCl2 at 1273 K. The results of this study showed the feasibility of the new Ti recycling process. The feasibility of a new Ti coating method based on the dispropotionation of

TiCl2 is also discussed from some of the results obtained in the preliminary experiments.

3:15 PM
Modeling Beta-Transus Temperature of Titanium Alloys: *N. S. Reddy*[1]; Chan Hee Park[2]; Chong Soo Lee[2]; [1]GIFT, POSTECH, Pohang, Korea; [2]Department of Materials Science and Engineering, POSTECH

Beta transus temperature is the basic reference point for treatment in titanium alloys. Therefore, it is desirable to determine this temperature for a given alloy accurately, especially for some near-a alloy whose processing window is narrow. The beta transus is sensitive to chemical composition and the relationships between them are complex and nonlinear. An artificial neural network (ANN) model was developed to simulate the nonlinear relationship between the alloying elements and beta transus temperature. By performing sensitivity analysis on ANN model, the individual and the combined influence of alloying elements on beta transus was achieved. The optimum percentage of composition for the desired beta transus was calculated by using genetic algorithms. The results are in agreement with experimental data. Explanation of the calculated results from the metallurgical point of view is attempted. The model can be used as a guide for further alloy development.

3:40 PM Break

3:55 PM
Study of Ti-6Al-4V in Liquid State by Electrostatic Levitation: *John Li*[1]; Won-Kyu Rhim[1]; William Johnson[1]; [1]Caltech

Some thermophysical properties of liquid Ti-6Al-4V were measured around the melting temperature by the Electrostatic Levitation. The properties include the specific heat, the total hemispherical emissivity, the heat of fusion, the density and the thermal expansion coefficient with 280 ° K of undercooling in liquid state. Over 1661 ~ 1997 ° K the ratio of the constant pressure heat capacity and the total hemispherical emissivity for liquid phase can be expressed by $C_p/\varepsilon_T = 3064 + 0.1291(T - T_m)$ J/kg/K with the melting temperature T_m = 1943 ° K. The heat of fusion has been measured to be 300 kJ/kg. Liquid density over 1661 to 1997 ° K can be expressed by $d(T) = 4123 - 0.254\ (T - T_m)$ kg/m^3, and the corresponding volume expansion coefficient is $\alpha = 6.05 \times 10^{-5}\ K^{-1}$ near T_m.

4:20 PM
Laser Additive Manufacturing of Titanium for Orthopedic Implants: *James Sears*[1]; Dana Medlin[1]; Jacob Fuerst[1]; [1]South Dakota School of Mines & Technology

Increasing the lifespan of implants by improving fixation of the medical device in bone tissue, through improved osteointegration, can increase patient health and decrease medical costs by reducing the need for revision surgeries on an implant. Initially a scaffolding designed to more accurately match the porosity of cortical bone was deposited on a Ti-6Al-4V substrate with a Nd: YAG laser piped through a 600µm fibre and finely screened Ti-6Al-4V or Ti-15Mo powder in an argon atmosphere. Subsequent testing has been performed using a new M-LAM system that employs a 10 µm fiber with six degrees of freedowm motion. Using very fine Ti-6Al-4V powder, structured surfaces were deposited onto a like substrate demonstrating surface features as low as 100µm with minimal substrate distortion and a heat affected zone of less than 200µm deep.

4:45 PM
Laser Beam Welding of ATI 425 Titanium: *Paul Edwards*[1]; Todd Morton[1]; Greg Ramsey[1]; [1]The Boeing Company

Laser Beam Welding of the low cost alloy ATI 425 was performed on 2 mm gage butt joints. This new alloy could be used in place of standard Ti-6Al-4V for a variety of lower cost solutions. Demonstration of its fusion weldability with laser welding is of particular interest because it is a near net shape process, capable of high welding speeds, which will further enable low cost manufacturing options. It was found that ATI-425 could be successfully welded using a fiber laser at speeds over 2 m/min. Results of the laser welding process development along with the resulting metallographic and mechanical property evaluations will be presented.

5:10 PM
Heat Treatments for Friction Stir Welded Ti-6Al-4V: *Paul Edwards*[1]; Marc Petersen[1]; [1]The Boeing Company

Friction Stir Welding is a solid state joining process which can be used to fabricate near net titanium structures at a reduced cost compared to traditional manufacturing processes. To date, Friction Stir Welding of titanium 6Al-4V has been demonstrated in butt welds, corner welds, T-welds and complex contour structures from 1.5 to 12 mm in thickness. Heat treatment processes for standard fusion welding techniques in titanium are well established, but the optimal heat treatment for Friction Stir Welded titanium has not been evaluated. In this study, 6 mm thickness titanium 6Al-4V butt welds were subjected to heat treatments ranging from 700 to 900 C. Results of the metallographic analysis for each heat treatment condition will be presented in addition to tensile and fatigue properties.

Electrode Technology for Aluminum Production: Anode Baking/Anode Properties

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee
Program Organizers: Ketil Rye, Alcoa Mosjøen; Morten Sorlie, Alcoa Norway; Barry Sadler, Net Carbon Consulting Pty Ltd

Wednesday PM — Room: 616
February 17, 2010 — Location: Washington State Convention Center

Session Chair: Gudrun Saevarsdottir, Reykjavik University

2:00 PM Introductory Comments

2:05 PM
On the Logistics of Rebuilding an Anode Baking Furnace while Maintaining Operation: *Richard Coulombe*[1]; David Machado[1]; John Ferguson[2]; Darren Carle[2]; [1]Hatch and Associates; [2]Portland Aluminium

During 2008, Portland Aluminium Smelter refurbished one of its two anode baking furnaces. The works included replacing the insulation and dense refractory with a new design to allow larger anodes within the existing tub, introducing a new state-of-the-art firing system, replacing the waste gas main and building a new scrubber. This refurbishment was done on-the-run, with ongoing production on three of the four fire trains on the furnace, thereby minimising the quantity of replacement anodes required to maintain smelting operation. This paper will elaborate on the project management, safety aspects and logistics required to achieve a successful rebuild, whilst maintaining baked anode quality.

2:30 PM
Specific Energy Consumption in Anode Bake Furnaces: Felix Keller[1]; *Peter Sulger*[1]; Markus Meier[1]; Dagoberto Schubert Severo[2]; Vanderlei Gusberti[2]; [1]R&D Carbon Ltd.; [2]PCE Ltda.

In anode baking, specific energy consumption is one of the important cost elements. When ordering a new furnace the buyer therefore asks for guarantees regarding specific energy consumption. Typically such guarantees are asked for from the supplier of the process control system. This approach is inappropriate, as will be explained in this document. Specific energy consumption is a function of numerous variables of which most are outside the sphere of influence of the process control system supplier. This document discusses the main factors influencing the specific energy consumption for anode bake furnaces.

2:55 PM
Desulphurisation Control during Anode Baking, Its Impact on Anode Performance and Operational Costs-Alba's Experience: *Hameed Abbas*[1]; Khalil Khaji[1]; Daniel Sulaiman[1]; [1]Aluminium Bahrain

During year 2006, carbon dusting was noticed in the pots of lines 4 and 5, operating at 335 and 340 kA current. One of the main parameters for carbon dusting in the pots is the CO2 dust loss which is influenced by the degree of anode desulphurisation which again is dependent on the level of anode baking. Alba developed an approach to optimize the anode baking level to control the desulphurisation of anodes to resolve the carbon-dusting problem. The approach shows that optimization of anode baking could be an effective way to resolve the carbon dusting in pots operating at high kA currents. In addition, there are benefits of reduced natural gas consumption, SO2 emissions. There is significant impact on the increase in flue wall refractory life. The paper describes the approach, and presents the results of the work on control of anode desulphurisation.

3:20 PM Break

3:35 PM
Development of a New Improved Dry Alumina Scrubber for Emission Control from Anode Bake Furnaces: *Paulo Douglas Vasconcelos*[1]; André Mesquita[2]; [1]Albras Alumínio Brasileiro S.A; [2] Solve Engenharia Ltda

The alumina-based dry scrubbing for emission control from potrooms in the aluminum industry is nowadays the standard process, and some different technologies are commercially available in the market. However, the presence of tar and SO2 together the emission of fluorides still represent a challenge for an efficient dry scrubber using alumina as adsorbent. This work presents the development of a new improved alumina-based dry fluidized bed scrubbing for emission control from anode bake furnaces. The development is carried-out from an experimental prototyping testing to a real pilot plant. This system uses a cooling tower, an in-duct initial adsorption process, and a fluidized bed and bag house for secondary and final adsorptive process, in order to assure the desulfurization, and the elimination of tar and fluorides emission. The results from a pilot plant installed at Albras smelter for emission control from an anode bake furnace are presented.

4:00 PM
Baked Anode Density Improvement through Optimization of Green Anode Dry Aggregate Composition: *Khalil Khaji*[1]; Hameed Abbas[1]; [1]Aluminium Bahrain

At Alba, green anodes were manufactured as per the dry aggregate composition recipe given by the technology suppliers. For given set of raw materials, paste plant process and equipment parameters the dry aggrgate composition was giving baked anode density of 1.565-1.570 g/cm3. Pot rooms gradually increased line current to increase aluminium metal production. Therefore there was need to improve baked anode density, net carbon consumption so that butts thickness at increased line current will be maintained. With in-house research, baked anode density of 1.600 g/cm3 was achieved. This was achieved by optimization of dry aggregate composition. The paper describes the work done on the optimization of dry aggregate composition and the results achieved over a period of two and half years.

4:25 PM
Characterization of Surface Topography on Carboxy Reactivity Residue: *Stein Rørvik*[1]; Lorentz Petter Lossius[2]; Hogne Linga[2]; Arne Petter Ratvik[1]; [1]SINTEF Materials & Chemistry; [2]Hydro Aluminium

The ISO 12988-1 method for determinating carboxy reactivity of anodes has widespread use in the aluminium industry. In this test, an anode core sample is exposed to CO_2 at 960°C for 7 hours. The relative amount remaining sample and accumulated dust is then measured. Visually, some samples show distinct selective reactivity, but there is currently no quantification of the degree of this selective reactivity (except for its indirect impact on sample weightloss and dust produced). To address this, an apparatus and a method were developed to quantify the surface topography of the tested samples. The method is based on automatically taking a picture-series of a back-lighted sample rotated in small increments using a computer controlled motor. A computer program then applies image analysis to the sample profile in the pictures to create a 3D reconstruction of the surface. This is then compared to carboxy reactivity and other anode properties.

Federal Funding Workshop

Wednesday PM — Room: 602
February 17, 2010 — Location: Washington State Convention Center

4:30 PM
Materials Research Support at the Office of Basic Energy Sciences: *John Vetrano*[1]; [1]Program Manager, Division of Materials Science and Engineering, Office of Basic Energy Sciences, Office of Science, Department of Energy

John Vetrano will give an overview of the fundamental materials research activities at the DOE office of Basic Energy Sciences (BES). BES Supports basic research in materials science, chemistry, geo-sciences and biosciences, as well as the construction and operation of nearly two dozen major scientific user facilities, including the nation's large synchrotron radiation light sources, neutron scattering facilities, electron-beam microscopy centers, and nanoscale science research centers. The major emphasis of the materials science and engineering program at BES is on fundamental experimental and theoretical research that provides the foundations for the discovery and design of new materials with novel functions and properties. Disciplinary areas supported include: Materials physics; condensed mater physics; mechanical behavior; materials chemistry; biomolecular materials; x-ray-, neutron-, and electron-scattering sciences; and related disciplines where the emphasis is on the science of materials. Knowledge gained in the program is aimed at providing the scientific basis for a clean, sustainable, and secure energy future through materials innovation. The presentations will highlight specific new research opportunities, including basic research on nanoscale science, hydrogen economy, solar energy utilization, advanced nuclear energy system, superconductivity, solid-state lighting, and other research areas. Inquiries can be directed to John.Vetrano@science.doe.gov.

5:00 PM
Materials Research Support at the National Science Foundation: *Alan J. Ardell*[1]; [1]Program Director, Metals and Metallic Nanostructures Division of Materials Research, Directorate of Mathematical and Physical Sciences, National Science Foundation

The NSF/DMR perspective on materials research and education will be presented. NSF invested ~$400M in FY09, supporting people, ideas, and instrumentation primarily through awards to the nation's colleges and universities: that figure was supplemented by the ARRA allocation of ~$107M. Apart from DMR, there is also substantial support for materials and materials-related research and education from other programs in NSF. Specific new opportunities – including the 3+ year-old program in biomaterials and the recent SOLAR and EFRI initiatives – will be described. There are also avenues for collaborative research, nationally and internationally, via different types of special funding programs (e.g. MRSEC). The projects supported by the MMN program in FY09, including the impact of the ARRA funds, and the budgetary outlook for FY10 will be described. General information on all the programs in DMR can be found on the DMR Web page: <http://www.nsf.gov/mps/divisions/dmr/>.

5:30 PM
The Technology Innovation Program (TIP): *Funding Innovative Research for Critical National Needs*: *Michael A. Schen*[1]; [1]Scientific Advisor to the Director, Technology Innovation Program, NIST

Located at the National Institutes of Standards and Technology (NIST) in Gaithersburg, Maryland, TIP has the purpose to help U.S. businesses, institutions of higher education, and other organizations—such as national laboratories and nonprofit research institutes—support, promote, and accelerate innovation in the United States by funding high-risk, high-reward research in areas of critical national need. This presentation will familiarize participants with the mission, objectives, and methods of the TIP program, provide insights on areas of nation attention being examined by the program, and outline TIP's activities and possible competition for 2010. Information about four areas of possible interest for future TIP solicitations may be found at http://www.nist.gov/tip/wp_cmts/index.html. TIP also has a booth as part of the TMS Annual Meeting where representatives are available for discussion.

General Abstracts: Electronic, Magnetic and Photonic Materials Division: Session I

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Alloy Phases Committee, TMS: Biomaterials Committee, TMS: Chemistry and Physics of Materials Committee, TMS: Electronic Materials Committee, TMS: Electronic Packaging and Interconnection Materials Committee, TMS: Nanomaterials Committee, TMS: Superconducting and Magnetic Materials Committee, TMS: Thin Films and Interfaces Committee, TMS: Energy Conversion and Storage Committee
Program Organizers: Long Qing Chen, Pennsylvania State University; Sung Kang, IBM Corporation; Mark Palmer, Kettering University

Wednesday PM Room: 308
February 17, 2010 Location: Washington State Convention Center

Session Chair: To Be Announced

2:00 PM Introductory Comments

2:05 PM
Multiferroic Fibers by Electrospinning: *Shuhong Xie*[1]; Jiangyu Li[1]; [1]University of Washington

In this paper, we report a strategy for synthesize multiferroic fibers at nanoscale. Three kinds of multiferroic fibers are synthesized by a sol-gel process and electrospinning, which include composite multiferroic CoFe2O4-Pb(Zr0.52Ti0.48)O3, NiFe2O4-Pb(Zr0.52Ti0.48)O3,and single phase BiFeO3 fibers. After being calcined, the diameters of multiferroic fibers are in the range from 100 to 300 nm. CoFe2O4-Pb(Zr0.52Ti0.48)O3, NiFe2O4-Pb(Zr0.52Ti0.48)O3 composite nanofibers are obtained by calcined in air. However, pure perovskite BiFeO3 nanofibers are obtained by using Ar as protective atmosphere. The spinel structure of CoFe2O4, NiFe2O4 and pervoskite structure of Pb(Zr0.52Ti0.48)O3, BiFeO3 are verified by X-ray diffraction and high resolution transmission electron microscopy. Transmission electron microscopy indicate that multiferroic nanofibers are composed of rather dense nanocrystalline grains with differnt nanograin size. The piezoresponse force microscopy (PFM) is used to confirm the ferroelectricity of multiferroic nanofibers. Ferromagnetism of multiferroic fibers are also confirmed by vibrating sample magnetometer (VSM) measurement.

2:25 PM
High-Temperature Thermoelectric Behaviors of Highly Dense Polycrystalline Nonstoichiometry TiOx Ceramics: Yong Liu[1]; Jinle Lan[2]; Bo-Ping Zhang[3]; *Hongmin Zhu*[1]; [1]School of Metallurgical and Ecological Engineering, University of Science and Technology Beijing; [2]State Key Laboratory of New Ceramics and Fine Processing, Department of Materials Science and Engineering, Tsinghua University; [3]School of Materials Science and Engineering, University of Science and Technology Beijing

Polycrystalline nonstoichiometry TiOx (x=1.6, 1.7, 1.8 and 1.9) ceramics with high density were prepared by a spark plasma sintering process at 1373 K using TiO2 and TiO as starting materials. The temperature dependences of the electrical conductivity, Seebeck coefficient, and power factor have been investigated. The results indicate that the electrical conductivity of all the samples is in the range of a semiconductor transport behavior(51 Scm-1 ~360 Scm-1), increases with temperature increasing, and decreases with oxygen content increasing. All samples show high negative Seebeck coefficients (-50~-375 μV/K), reveals that the primary carriers in these ceramic samples are electrons. Power factor of all samples increased with temperature increasing. The obtained TiO1.6 ceramic shows better thermoelectric properties and the maximum power factor ~5×10-4 Wm-1K-2 has been obtained at 873K in the air, which can be a promising candidate of n-type material for high-temperature thermoelectric application.

2:45 PM
Microstructure and Temperature Dependence of Ferroelectric Properties of Bi(Mgtio3)-PbTiO3 Ceramics: *Seema Sharma*[1]; D. Hall[2]; [1]Magadh University; [2]Materials Science Center

Ceramics in the (1-x) Bi(Mg0.5Ti0.5)O3-(x)PbTiO3 perovskite system with =0.30,0.35 and 0.40 have been processed by conventional sintering (9500C) from ceramics powders synthesized by direct solid-state reaction of the constituent oxides. X-ray diffractograms reveal the transformation of crystal structure from rhombohedral to tetragonal for x=0.35 to 0.40. Ferroelectric hysteresis curves show the transition from ferroelectric to antiferrolectric state with respect to temperature upto 1500C at an applied electric field of 6kV/mm. As the PbTiO3 content increases in the composition, the ferroelectric curves become less constricted in the central region. This effect is the most pronounced at x=0.40 and is quite expected one, since PbTiO3 being a ferroelectric material, the curves tend towards the conventional ferroelectric curves. Diffusivity (γ) study of phase transition in these compounds provided values between 1 and 2 indicating the variation of degree of disorderness in the system.

3:05 PM Break

3:35 PM
Bio-Inspired Methods to Self-Assemble 3D Micro-/Nano-Structures for Energy Harvesting: Huan Li[1]; Xiaoying Guo[1]; *K. Jimmy Hsia*[1]; Ralph Nuzzo[1]; [1]University of Illinois at Urbana-Champaign

Often used in nature, self-assembly at the micro- and nanoscales is a powerful tool to construct complex 3D structures from planar sheets. Water, among all materials, plays a critical role in many self-assembling processes. In particular, these processes often involve surface phenomena, such as capillary interactions and surface adhesion. In the current work, we demonstrate that mechanics can indeed be a useful tool to help understand surface phenomena-driven self-assembly by considering the self-assembly of a 3-D photovoltaic device made of patterned, thin silicon sheets. A model is developed to identify the mechanisms controlling the behavior of these processes. Critical parameters emerge naturally from the analysis which can be used to guide the device formation and manufacturing of nanoscale components.

3:55 PM
Monitoring Electrode Degradation in Lithium Ion Batteries Using Acoustic Emission: *Kevin Rhodes*[1]; Claus Daniel[2]; Nancy Dudney[2]; Edgar Lara-Curzio[2]; [1]University of Tennessee; [2]Oak Ridge National Laboratory

Lithium ion batteries for large scale applications such as vehicles and stationary energy storage face the challenge of being safe, powerful, reliable, and cost effective. To fulfill the requirements and understand failure new characterization techniques must be developed for guidance to new materials with improved performance. Composite electrodes with various types of active materials, including silicon and LiCoO2, were charge cycled in lithium ion half cells while monitoring acoustic emission. Both constant current and cycled voltage experiments were performed. Readily identifiable waveforms were recorded that are attributed to the degradation of active materials as observed cycled electrodes by SEM. This technique is being used to guide the development of improved materials capable of higher charge rates and greater cycle life.

4:15 PM
$CuInSe_2$/Si Heterojunctions for Photovoltaic Applications: *Okechukwu Akpa*[1]; Shaik Shoieb[1]; Kalyan Das[1]; [1]Tuskegee University

Growth and characterization of $CuInSe_2$ (CIS) thin films deposited on Si, for the purpose of forming heterojunctions to investigate the suitability of the material system for high efficiency solar cells, is reported here. Deposition was obtained by rf magnetron sputtering using a stoichiometric CIS target. As CIS and Si are closely lattice matched, large grain polycrystalline films were obtained. Rutherford backscattering spectroscopy (RBS) indicated that these CIS films have a composition of $Cu_{1.05}In_{1.04}Se_{2.5}$. Circular diodes were fabricated and the current-voltage characteristics of these diodes indicated that reasonable quality p-n junctions were obtained. The forward current of these devices increased by three orders of magnitude from 0.003 to 2.65 mA at a bias of 2 V when illuminated with a 75 watt halogen lamp and this strong response to illumination indicates that the material system has a high potential for use as solar cells.

4:35 PM
The Multi-Level Switching PRAM Device Using Stacked Phase Change Materials Structure: *Sung-Hoon Hong*[1]; Heon Lee[1]; [1]Korea University

Phase change random access memory (PRAM) is considered to be the most promising next generation non-volatile memory. Recently, multi-level switching of PRAM device has been studied for high density memory device. In this study, multi-level switching phase change memory, which has stacked phase change materials (PCMs) structure, was suggested. As stacked PCMs, Ge2Sb2Te5/ AgInSbTe, Ge2Sb2Te5/ GeTe, In2Se3/ Ge2Sb2Te5 PCMs were used. The 200nm stacked PCMs structure nano-pillar device was fabricated using NIL and the electrical property was studied using c-AFM connected a pulse generator and voltage source. In case of Ge2Sb2Te5/ GeTe and In2Se3/ Ge2Sb2Te5 PCMs stacked structure PRAM device, multi-level switching was observed.

General Abstracts: Light Metals Division: Session II

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee, TMS: Magnesium Committee, TMS: Recycling and Environmental Technologies Committee, TMS: Energy Committee, TMS: Aluminum Processing Committee

Program Organizers: Alan Luo, General Motors Corporation; Eric Nyberg, Pacific Northwest National Laboratory

Wednesday PM February 17, 2010 — Room: 607 — Location: Washington State Convention Center

Session Chair: Eric Nyberg, Pacific Northwest National Lab

2:00 PM
Enhanced Resistance of Ti-Alloys against Environmental Attack by a Combined Al- and F-Treatment: *Alexander Donchev*[1]; Michael Schütze[1]; Rossen Yankov[2]; Andreas Kolitsch[2]; [1]DECHEMA; [2]FZD

Titanium alloys cannot be used at elevated temperatures above approximately 500°C because of their limited environmental stability. Several ways have been investigated so far to improve the environmental stability of Ti-alloys e.g. coatings but these attempts in a majority of cases have not been really successful. A new way to improve the performance of these alloys is the combination of Al-enrichment in the surface zone plus additional fluorine treatment. The Al-enrichment leads to the formation of intermetallic phases. These phases improve the oxidation resistance of Ti-alloys but not to a sufficient extent. An additional fluorine treatment on top of the Al-enriched surface leads to the formation of a stable alumina scale due to the fluorine effect. In this paper results from oxidation and other tests performed on Ti-samples without any treatment, with single Al- or F-treatment and with a combination of both are presented and the results are discussed.

2:20 PM
Fabrication of Aluminum Foam with New Stabilizer Composited by Fly Ashes and Short Copper-Coated Carbon Fibers: *Pei-hong Chen*[1]; Hong-jie Luo[1]; Lei Wang[1]; Yong-liang Mu[1]; [1]Northeastern University

Closed-cell Al foam contained fly ashes and short copper-coated carbon fibers as composite stabilizer was successfully prepared by melt direct foaming process. The scanner at the resolution of 300dpi, SEM and EDX were used to investigate the macro and microstructure of foamed samples. The results show that vertical density gradient is reduced and cell sizes are well-proportioned. Fly-ash particles are located mainly at the edges of cell walls and Plateau borders, and short copper-coated carbon fibers exist inside cell walls. Over a very large number of trials, foam stability is improved greatly by the composite stabilizer consisting of 3.0wt.% copper-coated carbon fibers and 2.0wt.% fly ash particles fibers.

2:40 PM
Fundamental Materials-Design Limits in Ultra Light-Weight Mg-Li Alloys Determined from Quantum-Mechanical Calculations: *Martin Friak*[1]; William Counts[1]; Dierk Raabe[1]; Joerg Neugebauer[1]; [1]Max Planck Institute for Iron Research

Quantum-mechanical calculations are becoming increasingly useful to engineers interested in designing new alloys because these calculations are able to accurately predict basic material properties only knowing the atomic composition of the material. In this paper, fundamental physical properties (formation energies, elastic constants) of 11 bcc Mg-Li compounds are calculated using density-functional theory (DFT) and compared with experimental data. These DFT-determined properties are in turn used to calculate engineering parameters like (i) specific Young's modulus (Y/rho) or (ii) bulk over shear modulus ratio (B/G) differentiating between brittle and ductile behavior. The engineering parameters are then used to identify alloys that have optimal mechanical properties for light weight applications. An Ashby map containing Y/rho vs. B/G shows that it is not possible to increase both Y/rho and B/G by changing only the composition or local order of a binary alloy (W. A. Counts et al., Acta Mater 57 (2009) 69-76).

3:00 PM
Material Selection for the Lining of Aluminum Holding and Melting Furnaces: *Andy Wynn*[1]; John Coppack[1]; Tom Steele[1]; [1]Thermal Ceramics

The range of monolithics available for lining Aluminum holding and melting furnaces is extensive and product selection can be confusing. Without appropriate material selection for the furnace lining, furnace performance will be compromised. An understanding of monolithic selection criteria is critical in providing efficient furnaces for processing Aluminum. This paper reviews operating conditions found in all key zones of a typical melting and holding furnace – Belly Band/Lower Wall, Hearth/Ramp (working face), Hearth/Ramp (substructure) and Superstructure. The test methods utilised by many of the large Aluminum producers for product selection are reviewed and areas where these test methods do not neccessarily reflect real operating conditions are highlighted. A range of monolithic materials are subjected to a representative program of approval testing. A package of monolithic technologies is proposed that will assist the furnace designer in selecting the best material available for each of the key furnace zones.

3:20 PM
Mechanical Properties and Precipitation Behaviors of Mg-Al-Sn and Mg-Zn-Sn Alloys: *Toyohiko Konno*[1]; JongBeom Lee[1]; Takahiro Ohya[1]; Hyeon-Taek Son[2]; Haguk Jeong[2]; [1]Tohoku University; [2]Korea Institute of Industrial Technology

In order to develop low-cost Mg alloys, we have examined age-hardening behaviors of Mg-Al-Sn (MAS) and Mg-Zn-Sn (MZS) alloys, with and without Mn addition, by means of a mechanical testing and microstructure characterization using transmission electron microscopy (TEM). For the MAS alloys, the ultimate strength (UTS) of an extruded Mg-9wt%Al-2wt%Sn alloy reached 390MPa. TEM observation indicated that plate-like Mg17Al12 precipitates having Burgers orientation relationship with the matrix are responsible for the strength. This alloy also exhibits age hardening behavior. For example, the peak hardness appears after 15-20 hrs of heat treatment at 473K. On the other hand, the UTS of the MZS alloys are on the order of 300MPa. It was found that the addition of Mn effectively make their grain size small. The precipitates are composed of the Mg2Sn and MgZn2 phases, and interestingly, the former often acts as a nucleation sites for the latter.

3:40 PM Break

4:00 PM
Microstructure and Composition Modifications in the Surface Layers of a Mg AZ80 Alloy Induced by Laser Melting: *Kemin Zhang*[1]; Jianxin Zou[2]; [1]Shanghai University of Engineering Science; [2]University of British Columbia

Laser surface melting has been applied on a cast Mg AZ80 alloy to improve its surface properties. The microstructure and composition modifications encountered in the surface layers were carefully investigated by using SEM, EDX and XRD techniques. The untreated alloy contains coarse grained Mg matrix, large sized Mg17Al12 intermetallic phase at grain boundaries and AlMn particles. Due to the melting followed by rapid solidification and cooling, a layer having graded microstructures and compositions formed. The Mg17Al12 phase was completely dissolved into the melted layer during melting and partially segregated as very fine particles during solidification in inter-dendritic areas. In contrast, the AlMn particles could not be fully dissolved at the bottom of the melted layer owing to their high melting point. The difference in the chemical composition and the thermal history at different depths has a strong impact on the segregation behaviours and hardness distribution in the melted layer.

4:20 PM
Multi Sensor Data Fusion for Aluminium Cell Health Monitoring and Control: *Håkon Viumdal*[1]; Ru Yan[2]; Morten Liane[3]; Bjørn Petter Moxnex[4]; Saba Mylvaganam[5]; [1]Telemark Technological Research and Development Centre (tel-tek); [2]Telemark University College; [3]Hydro, Primary Metal Technology; [4]Hydro Aluminium; [5]Telemark Technological Research and Development Centre (tel-tek) and Telemark University College

The prevailing aluminium electrolysis process demands steady-state conditions within narrow borders, to improve performance with respect to molten metal production per day, energy usage per kg of aluminium, current efficiency, CO_2 and flour-gas emissions etc. However, only the current and the cell voltage are obtained by on-line measurements. Many bath parameters are manually measured on a daily or even weekly basis. Innovating measurements of the bath temperature, the bath chemistry, the molten metal height and the height of the electrolyte would all be of substantial importance for the control regime. However, combining new measurements and soft sensors for estimating “unavailable” variables would improve both the monitoring and controlling tasks of the aluminium electrolysis process. This paper gives an overview of many online and off-line measurements and reports some new possible measurement scenarios with increasing potential for extensive, fast, efficient and even real-time data fusion. Finally some interesting examples of data fusion examples based on actual plant measurements covering many months are also included.

4:40 PM
Effect of Copper Coatings on the Interfacial between Short Carbon Fiber and Aluminum Matrix: *Yan Pengfei*[1]; Yao Guangchun[1]; Shi Jianchao[1]; Mu Yongliang[1]; [1]School of Materials and Metallurgy, Northeastern University

Short carbon fiber reinforced aluminum alloy matrix composites were prepared by stir casting. The fibers were coated copper by electroless plating and then characterized. The microstructure of the composites was observed by Optical Microscope, Scanning Electron Microscope (SEM) and XRD. The results show that copper coating prevents the harmful interfacial reaction between carbon fibers and aluminum matrix, and improves the wettability between the fibers and molten aluminum, and carbon fiber distributes homogenous in the aluminum matrix.

5:00 PM
Effect of Mg on Microstructure and Mechanical Properties of Copper-Coated Short Carbon Fiber Reinforced Aluminum Alloy Matrix Composite: *Yan Pengfei*[1]; Yao Guangchun[1]; Shi Jianchao[1]; Mu Yongliang[1]; [1]School of Materials and Metallurgy, Northeastern University

Copper coated short carbon fiber reinforced aluminum alloy matrix composites have been prepared with 0.3-1.5 wt% Mg as alloying addition by stir casting. Effect of Mg on the microstructure and mechanical properties of the composites was investigated. The microstructure was observed by scanning electron microscopy (SEM) and the results show that adding Mg can make the distribution of carbon fibers uniform in the composites, reduce laminated and agglomerated. Tensile test and hardness test were carried out, the results show that the tensile strength and the hardness of the composite is increased by 13% and 8% when Mg content is 0.9 wt%.

General Abstracts: Materials Processing and Manufacturing Division: Synthesis and Processing

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS/ASM: Computational Materials Science and Engineering Committee, TMS: Global Innovations Committee, TMS: Nanomechanical Materials Behavior Committee, TMS/ASM: Phase Transformations Committee, TMS: Powder Materials Committee, TMS: Process Technology and Modeling Committee, TMS: Shaping and Forming Committee, TMS: Solidification Committee, TMS: Surface Engineering Committee
Program Organizers: Thomas Bieler, Michigan State University; Corbett Battaile, Sandia National Laboratories

Wednesday PM — Room: 601
February 17, 2010 — Location: Washington State Convention Center

Session Chair: To Be Announced

2:00 PM
Innovative and Integrated Technologies for the Development of Aeronautic Components: *Nicola Gramegna*[1]; Franco Bonollo[2]; Emilia Della Corte[1]; Fabio Grosselle[2]; Marco Cocco[3]; [1]ENGINSOFT; [2]University of Padova - DTG; [3]AVIO S.p.A.

The “design innovation program” lies in the development and integration, since the very first steps, of all those aspects related with component life cycle, from manufacturing till end_of_life, in order to meet the requirements of a greater product quality, of a more and more comprehensive knowledge about the component potential, of a cost and TTM (Time To Market) reduction. In particular, the knowledge about the mechanical properties, coming from the manufacturing process, contributes to the improvement of the component performance and reliability, to exploit the synergies of the departments involved in the project and to maximize the suppliers collaboration.In such perspective, light alloy components for aeronautic sector play an important role. Propulsive systems consist of complex and diversified parts that require a structural design in the non-linear and fatigue fields, to be also integrated in the main manufacturing aspects: the casting process and the subsequent heat treatment.

2:20 PM
Selective Laser Sintering of Magnesium Powder for Fabrication of Compact Structures: *Ng Chi Chung*[1]; [1]The Hong Kong Polytechnic University

In past decades, considerable research effort has been reported in the area of direct metal laser sintering (DMLS). However, rarely work has previously been found on the laser sintering of magnesium powder. The novelty of the present research lies in the fabrication of compact structures by laser sintering of magnesium powder using a Nd:YAG laser. The laser sintering of single tracks and single layers of magnesium powder were carried out for demonstrating the process feasibility and for examining the influences of several processing parameters (laser power, scan speed and repetition rate) on microstructural characteristics and mechanical properties of the final sintered structures. The experimental results give valuable information about geometrical features and microstructural evolution of magnesium powder under a Nd:YAG laser irradiation, which would facilitate the fabrication and controllability of compact structures by deliberating the associated effect of different processing parameters for fabrication of structural parts in transportation industries.

2:40 PM
Novel Lead-Free Bronze Bearing Materials Produced by Powder Metallurgy Processing: *Greg Vetterick*[1]; Iver Anderson[1]; Matthew Besser[2]; [1]Ames Laboratory and Iowa State University; [2]Ames Laboratory

Leaded bronze alloys such as Cu-10Sn-10Pb (wt.%) are utilized effectively in tribological systems that are prone to lubrication starvation. These Cu-based leaded alloys typically exploit the insolubility of Pb in Cu to create soft phase pockets in the microstructure on solidification of a chill casting or a gas atomized powder. Properly distributed throughout the bearing, free Pb provides a low shear solid lubricant for sliding interfaces. However, the toxicity of Pb necessitates the development of alternatives for the soft Pb phase. The current work explores replicating the desirable microstructure of leaded bronze by utilizing powder metallurgy processes. Impregnation of a bronze matrix microstructure with Pb-free soft alloys shows considerable promise as a bearing alloy production method. Microstructural analysis and tribological evaluation of the resulting composite bearings helped verify adequate performance as a Pb-free bearing system. Supported by Sauer-Danfoss Inc. as work for others through Ames Laboratory Contract No. DE-AC02-07CH11358.

3:00 PM
Microstructural Evolution of Cu, Ni and Al Powder Particles Processed by Cold Spray: *Yu Zou*[1]; Ahmad Rezaeian[1]; Eric Irissou[2]; Jean-Gabriel Legoux[2]; Jerzy Szpunar[1]; Stephen Yue[1]; [1]McGill University; [2]National Research Council Canada (NRC)

Cold spray is a relatively new coating technology by which coatings can be produced using high-velocity impact of powder particles without significant heating introduced. Micron-sized pure Cu, Ni and Al powder particles were processed by the cold spray, respectively. Microstructural evolutions of these particles were investigated using electron backscatter diffraction and transmission electron microscopy. The results show that non-uniform microstructures with elongated grains/subgrains in the size of microns, equaxied grains in sub-microns and nanocrystalline grains appear in as-sprayed materials. Moreover, deformation twins in nano-scale are observed in the cold sprayed Cu. Formation of these structures is explained by high strain-rate deformation with the dynamic recovery/recrystallization in the complex thermo-mechanical process during cold spraying.

3:20 PM
Recent Trends in Cold Spray Technology: *Julio Villafuerte*[1]; Bert Jodoin[2]; [1]Centerline Windsor Ltd; [2]University of Ottawa

Cold spray, emerged as a practical technology in the 1980’s from the Institute of Theoretical and Applied Mechanics of the Russian Academy of Sciences in Novosibirsk. Almost twenty years later, interest on this technology has grown exponentially. Today, cold spray is known as a solid-state spraying process where materials are not melted but simply propelled in a supersonic stream against the substrate to produce bonding; the advantage being the ability to produce fully dense deposits that are free of oxidation, tensile residual stresses and other thermal effects inherent to conventional thermal spray. Since the year 2000, a number of commercial cold spray technologies have become available. Today, they can be seen serving in applications including corrosion protection, restoration, repair, additive manufacturing, and others. This paper describes the process working principles, its advantages and challenges. It also presents the state of the art of the technology.

3:40 PM Break

4:00 PM
Introduction of High-Throughput, Commercial Application, Spark Plasma Sintering (SPS) Technology: *Robert Aalund*[1]; [1]Thermal Technology

Spark Plasma Sintering, and similar, technologies have been used in R&D and academically for compacting advanced ceramics, powder metals, and cermets for more than two decades. And SPS remains a highly sought-after research and development tool, because of its high speed processing, particle bonding attributes, and impressive material properties capabilities. Though there have been some attempts to apply this incredible technology to specific commercial projects, they remain largely unknown and are commonly veiled in a shroud of secrecy.This discussion is about removing the veil and looking closely at several examples of how SPS can be used commercially, today. We will review several equipment processing approaches designed around several types of product, including estimated throughput, operational costs, and tooling design. We will also discuss some of the limitations of SPS with regard to commercial applications.

4:20 PM
Thermo-Mechanical Behavior of Chemically Bonded Phosphate Ceramic Composites Reinforced with Graphene Nanoplatelets: A Substantial Material Improvement toward Structural Applications: *H. A. Colorado*[1]; C. Hiel[2]; H. T. Hahn[3]; [1]University of California, Los Angeles and Universidad de Antioquia; [2]Composite Support and Solutions Inc.; [3]University of California, Los Angeles

Mechanical properties and microstructures of a chemically bonded phosphate ceramic (CBPC) and its composite with 1.0 wt% graphite nanoplatelets (GNPs) reinforcement have been investigated. The GNPs were functionalized by different procedures including acid treatment and dried oxidation. Three different mixing techniques and different process parameters are evaluated. Microstructure was identified by using optical and scanning electron microscopes, x-ray micro tomography, and X-ray diffraction. In addition, weight loss of the resin at room temperature and pH were studied. The microstructure characterization shows that CBPC is a composite itself with several crystalline (wollastonite and brushite) and amorphous phases. SEM and micro tomography show a homogeneous distribution of crystalline phases. Bending strength of the composite material was increased from less than 10 Mpa (reported results) to more than 20MPa.

4:40 PM
Kinetics of Lamellar Decomposition in U-Nb Alloys: *Robert Hackenberg*[1]; Heather Volz[1]; Pallas Papin[1]; Ann Kelly[1]; Robert Forsyth[1]; Robert Dickerson[1]; Tim Tucker[1]; [1]Los Alamos National Lab

Lamellar decomposition products result when U-Nb alloys are transformed between about 300C and the 650C monotectoid temperature. The kinetics of these cellular precipitation reactions are of interest since the resulting microstructures give undesirable properties. Detailed kinetic studies of these reactions were undertaken in isothermally transformed U-5.6 wt% Nb and U-7.7 wt% Nb alloys. The volume fractions, growth rates, interlamellar spacings, and phase compositions of the initial discontinuous precipitation as well as the succeeding discontinuous coarsening reactions were investigated via light microscopy, X-ray diffraction, SEM, and TEM. These results will be compared with theory. Attention will be paid to the rates and degrees to which these various aging reactions drive the system toward its final equilibrium state.

5:00 PM
Synthesis and Microstructure of TiC/TiN Porous Ceramic Composites Processed via HYSYCVD/Direct Nitridation: *Jose Flores-Garcia*[1]; Martin Pech-Canul[1]; [1]Centro de Investigacion y de Estudios Avanzados del Instituto Politecnico Nacional

The effect of varying oxygen content in the nitrogen atmosphere during successive stages of vapor infiltration on the microstructural evolution and physical properties of TiC/TiN porous ceramic composites was investigated. Composites were processed via the hybrid precursor system chemical vapor deposition (HYSYCVD) and direct nitridation (DN) routes. TiCp porous preforms were infiltrated in subsequent stages: S1-1 and S1-2 at 1300°C for 70 min in high purity nitrogen (HPN); S2 at 1350°C for 120 min in ultra high purity nitrogen (UHPN). The composites were characterized by XRD, SEM, He picnometry, volume-measurement approach and immersion in Hg. The study was complemented with thermodynamic analyses using the FactSageTM program and databases. Results show that the presence of O2, NH3 and silicon-fluoride gaseous species throughout consecutive stages of processing affect the amount, morphology and distribution of TiN formed. Formation of TiN is ascribed to a combined effect of DN and HYSYCVD mechanisms.

5:20 PM
The Production of BCl_3 Gas from Mechanochemical Reaction Product Containing Elemental Boron and Magnesium Oxide: *Duygu Agaogullari*[1]; Ozge Balci[1]; Ismail Duman[1]; [1]Istanbul Technical University

The most preferred method in industrial production of boron trichloride (BCl_3) is from the carbon containing raw materials such as boron carbide (B_4C). In the proposed study, boron oxide (B_2O_3) was used as a cheap raw material. Firstly, elemental boron powder containing MgO was obtained as a result of mechanochemical synthesis of boron oxide (B_2O_3) and magnesium (Mg) powder mixture in a high-energy ball-mill (Spex 8000D Mixer/Mill) with a ball-to-powder weight ratio of 18:1. Then, chlorine gas (Cl_2) was passed through this intermediate product in a vertical quartz reactor heated to 650-1200°C by a tube furnace with SiC heating element. Cl_2 reacts only with free elemental boron while MgO powder behaves totaly inert. Thus, the formation of carbon-containing gaseous compounds ($COCl_2$) was prevented and high purity BCl_3 was obtained. Mechanochemically synthesized intermediate products were characterized by XRD and SEM whereas gaseous chlorination products were analyzed by FTIR.

5:40 PM
Cyclic Oxidation Behavior of Detonation Gun Sprayed Ni-20Cr Coating on a Boiler Steel at 900°C: *Gagandeep Kaushal*[1]; Harpreet Singh Saheet[1]; Satya Prakash[1]; [1]RIMT-Institute of Engineering & Technology

Detonation-gun spray technology provides the possibility of producing high quality coatings with significant adherence strength. In this study, Detonation gun spray technique was used to deposit Ni-20Cr coating on a commonly used boiler steel ASTM-SA213-T-22. The specimens with and without coatings were subjected to cyclic oxidation testing at an elevated temperature of 900°C to ascertain usefulness of the coating. Weight change data was evaluated to formulate the kinetics of the oxidation. The uncoated sample suffered intensive spallation along with a significant overall weight gain. The oxidation rate was found to reduce appreciably after the deposition of the coating as the overall weight gain was reduced by 91%. The exposed specimens were characterized by scanning electron microscopy and energy dispersive spectroscopy (SEM/EDS). It was observed that Detonation gun sprayed Ni-20 Cr coating was suitable to provide oxidation resistance to the given steel in the air environment.

Global Innovations in Manufacturing of Aerospace Materials: The 11th MPMD Global Innovations Symposium: Innovations in Primary and Secondary Forming - Aluminum, Magnesium, and Titanium Aluminides / Innovations in Machining and Joining

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Shaping and Forming Committee, TMS: High Temperature Alloys Committee
Program Organizers: Deborah Whitis, General Electric Company; Thomas Bieler, Michigan State University; Michael Miles, BYU

Wednesday PM — Room: 306
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Ron Wallis, Wyman Gordon; David Furrer, Rolls-Royce

2:00 PM
Simulating Hot Gas-Pressure Forming of Light Alloy Sheet Materials: *Eric Taleff*[1]; Louis Hector[2]; Paul Krajewski[2]; [1]The University of Texas at Austin; [2]General Motors Corp.

Superplastic forming and related hot gas-pressure forming technologies are used in the commercial production of light-alloy components for the transportation industries. Recent progress in simulation technologies, particularly the development of improved material constitutive models, provides for accurate predictions of these forming processes. This new capability now makes it possible to better design and optimize forming processes. Improved understanding of material response during hot forming also makes the integration of material design and optimization for light alloys possible. This presentation will summarize advances relevant to simulating the hot gas-pressure forming of aluminum and magnesium sheet materials and suggest how these may be introduced into the integrated computationalmaterials engineering paradigm.

2:20 PM
Stress Corrosion Behavior of Ti-Al-Nb Intermetallic Alloys Made from Accumulative Roll Bonding and Reaction Annealing: *Peng Qu*[1]; Mona El-Demellawy[2]; Viola Acoff[1]; [1]The University of Alabama; [2]American University of Cairo

The TiAlNb intermetallic compound has been considered as a potential structural material for the aircraft engine because of its light weight and excellent properties at elevated temperatures. In order to be a candidate material for the turbine engine, the TiAlNb alloy shall meet qualification requirements for the engine cleaning materials. In this paper, a ternary Ti-46Al-9Nb intermetallic alloy (at. %) was produced by accumulative cold roll bonding (ARB) followed by reaction annealing. The stress-corrosion test, which was according to the ASTM standard, was applied to the intermetallic alloy. The preliminary evaluation and metallographic inspection were performed by light microscopy and scanning electron microscopy. Cracks, especially the tension or compression cracks were examined in detail. It is predicted that the TiAlNb alloy in this study will have high stress-corrosion resistance. The relationship between number of ARB cycles and resistance will be evaluated. Key words: Ti-46Al-9Nb; cold roll bonding; stress-corrosion; intermetallics

2:40 PM
Study on the Asymmetric Cross Rolling of AZ31 Magnesium Alloy: *Bin Chen*[1]; [1]Shanghai Jiaotong University

The shear strain and its directions were thought to play an important role in severe plastic deformation (SPD) . Asymmetric rolling, however, has a shear deformation zone in the middle section of deformation zone. Accordingly, Asymmetric cross rolling, a new rolling method was developed by us. And its experiments have been conducted to investigate its effects on microstructure and mechanical properties of AZ31. The influencing factors such as velocity ratio of rolls, rolling route, rolling temperature were investigated. It was found that the shear strain of asymmetric cross rolling contributes to refinement of grain size. Samples rolled by asymmetric cross rolling have finer grain size than that rolled by common rolling.

3:00 PM
Fabrication of Dimensionally-Correct Sheet Metal Components Directly from T-6 Aluminum Alloys and Airframe Applications: Christian Weddeling[1]; Steven Woodward[2]; Bill Carson[3]; *Glenn Daehn*[2]; [1]Technische Universitat Dortmund ; [2]Ohio State University; [3]Cutting Dynamics

Aluminum airframe components are commonly produced from heat-treatable aluminum alloys by hydroforming in the soft condition and then heat treating them to the T-6 temper and then manually correcting the shape with hammers. Sometimes several form and anneal cycles are required to create the basic shape. A process is demonstrated wherein components can be made in a single step using a variant of rubber pad forming augmented with an electromagnetic calibration step using an inexpensive disposable electromagnetic actuator. This new process is amenable to single-part flow in the production environment and can dramatically reduce the time required to produce a quantity of parts. High dimensional accuracy is possible and the components maintain the peak-aged materials properties. This presentation will discuss in detail the important process variables.

3:20 PM
Role of Precipitates in the Actuation Behavior of NiTiPt High Temperature Shape Memory Alloys: *Shipeng Qiu*[1]; Santo Padula II[2]; Ron Noebe[2]; Raj Vaidyanathan[1]; [1]UCF; [2]NASA GRC

NiTiPt shape memory alloys hold promise in aerospace actuator applications as a result of their higher phase transformation temperatures when compared to binary NiTi. Recently, macroscopic thermomechanical testing has shown that $Ni_{29}Ti_{50}Pt_{21}$ samples aged at 500 °C for 5 h have better dimensional stability and higher work output when compared to non-aged samples. In order to assess the role of the resulting precipitates from the aging treatment on shape memory behavior, in situ neutron diffraction measurements during heating/cooling and mechanical loading were performed on aged and as-received $Ni_{29}Ti_{50}Pt_{21}$ samples. The influence of stoichiometry was additionally investigated by comparable experiments on a $Ni_{28.5}Ti_{50.5}Pt_{21}$ alloy. The role of precipitates in influencing texture evolution and internal strain development along with the phase transformation characteristics during deformation was quantitatively studied. The understanding presented offers new guidelines for processing NiTiPt alloys for high temperature aerospace applications.

3:40 PM Break

3:50 PM Invited
Analysis and Optimization of Aerospace Machining Processes: *Liangji Xu*[1]; [1]The Boeing Company

Commercial airframe manufacture has historically been machining intensive as metallic components are shaped into their required forms.Although there is significant movement to employ more composite materials in airframe manufacture, composite use has also driven the need to use more exotic metallic components. Materials such as titanium offer better thermal growth and corrosion characteristics but are more challenging to machine. Due to the high quantity of material that must be removed, it is critical to maintain high material removal rates in machining processes to minimize the manufacturing costs of the airframe parts.Material removal rates are often limited by design limitations of a machine tool, such as the spindle power and servo drive torque,as well as constraints imposed by the dynamic compliance of the machine structure and the cutting tools.Accurate calculation of the cutting forces generated during the machining process is essential in optimizing the process according to a machine tool's capability.

4:20 PM
Effect of Machining Processes on Low Cycle Fatigue Behavior of a Powder Metallurgy Disk Superalloy: *Jack Telesman*[1]; Pete Kantzos[2]; Tim Gabb[1]; Louis Ghosn[3]; [1]NASA GRC; [2]Honeywell International; [3]Ohio Aerospace Institute

A study has been performed to investigate the effect of various machining processes on fatigue life of configured low cycle fatigue specimens machined out of a NASA developed LSHR P/M nickel based disk alloy. Two types of configured specimen geometries were employed in the study. To evaluate a broach machining processes a double notch geometry was used with both notches machined using broach tooling. EDM machined notched specimens of the same configuration were tested for comparison purposes. Honing finishing process was evaluated by using a center hole specimen geometry. Comparison testing was again done using EDM machined specimens of the same geometry. The effect of these machining processes on the resulting surface roughness, residual stress distribution and microstructural damage were characterized and used in attempt to explain the low cycle fatigue results.

4:40 PM
Investigation a New Method for Produce Favorable Surface Integrity in as Machined Surface of Gamma Titanium Aluminide during HSM Machining: *Sajjad Kolahdouz*[1]; [1]Tehran Polytechnic (Amirkabir University of Technology)

Gamma titanium aluminide provides a peerless set of properties that can lead to substantial pay offs in aircraft engine applications. Regarded as a new material, machining of gamma titanium aluminide is much more difficult than machining Ti6A14V.Wile there have been many studies on the produce of gamma titanium aluminide intermetallics but studies that report the satisfactory condition when machining this component is restricted due to this reason use this material is limited. In this study HSM (high speed machining) and UHSM (ultra high speed machining) in dry and MQL (minimum quantity lubricant) condition of this component are studied by new tool. After that surface integrity and mechanism of chip formation and micro hardness were studied. These parameters and these results compare with electric discharge machining and grinding and fine polishing.

5:00 PM
Material Flow Forming the Shoulder Flow Zone Using Scroll Shoulder Tool during Friction Stir Welding of Thick Section Aluminum Alloys: *David Yan*[1]; Zhan Chen[1]; Guy Littlefair[1]; [1]AUT University

Scroll tool offers advantages of eliminating the tilted tool axis and performing non-linear thick section FSW with a simple machine. However, its shoulder flow zone forming mechanism, determining defect or defect-free weld formation, remains unidentified. A scroll tool was used to FSW thick aluminium plates under different conditions, thereby made a defect, non-defect and 'marker insert' welds for flow pattern investigation. It was observed that a layer-to-layer banded structure appears on the bottom section, but disappears on the top section of shoulder flow zone. Accordingly, shoulder flow zone forming mechanism was suggested. When tool pin is plunged into workpiece, workpiece material is extruded by the pin, and pushed up into the scroll groove forming the pick up material (PUM). During tool moving forward, the central portion of PUM is driven downward by the root portion of pin and then detaches from the tip portion of pin in a layer-to-layer manner.

5:20 PM
Effect of Welding Parameters on the Mechanical and Metallurgical Properties of Friction Stir Spot Welded 2024-T351 Aluminum Alloy: *Amin Maki*[1]; Masoud Goodarzi[1]; Shahram Kheirandish[1]; Mohamad Ali Safarkhanian[1]; [1]Iran University of Science and Technology

Friction Stir Welding (FSW) is less than fifteen years old and Friction Stir Spot Welding (FSSW) has just recently arrived on the scene. In this investigation, Friction stir spot welding was used to make lap joints on strips of 2024-T351 aluminum alloy sheets. The influence of tool rotational speed and tool holding time on bond formation and tensile shear strength of the resulting joints was determined. The weld microstructures varied significantly depending on tool rotational speed and tool holding time. Metallographic observations were performed by optical microscope. As results showed, wide of stir zone and heat affected zone and Thermo mechanical affected zone, increased by increasing of tool rotational speed and tool holding time. Micro indentation hardness data of base metal (BM), heat affected zone (HAZ), Thermo mechanical affected zone (TMAZ) and SZ were obtained. The HAZ is the softest region and stir zone hardness increased by increasing of tool rotational speed and tool holding time and then decreased. An optimum combination of parameters that maximizes joint strength was identified.

Hume-Rothery Symposium: Configurational Thermodynamics of Materials: Session VI

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Chemistry and Physics of Materials Committee
Program Organizers: Chris Wolverton, Northwestern University; Mark Asta, University of California, Davis; Gerbrand Ceder, Massachusetts Institute of Technology (MIT)

Wednesday PM Room: 212
February 17, 2010 Location: Washington State Convention Center

Session Chair: To Be Announced

2:00 PM Invited
Bulk and Surface Properties of Perovskites for Solid Oxide Fuel Cell Cathodes: *Dane Morgan*[1]; Yueh-Lin Lee[1]; [1]University of Wisconsin - Madison

Perovskites are the major class of materials used for modern solid oxide fuel cell (SOFC) cathodes and have the ability to catalyze the oxygen reduction reaction (ORR) on their surfaces and transport oxygen to the electrolyte through their bulk. Their effectiveness as a cathode is therefore intimately tied to their bulk and surface defect thermokinetics. In this talk we discuss some of the challenges and opportunities of using ab initio methods to determine perovskite thermokinetics for SOFC applications. In particular, we focus on LaBO3 (B= Mn, Fe, Co, and Ni) systems, their deviations from ideal defect behavior, and the impact of these deviations on stoichiometry and kinetics. We also consider how simple descriptors for the ORR can be established with ab initio methods for different SOFC materials.

2:30 PM Invited
Configurational Design of Functional Oxides: *Hisao Yamauchi*[1]; Maarit Karppinen[1]; [1]Helsinki University of Technology

Crystals of functional materials usually possess particular local structures from which the main part of functionality stems. For example, crystals of high-Tc superconductive copper oxides commonly have CuO2 planes where superconductivity occurs. Even without thorough understanding of the functionality mechanism it is wise to systematically categorize materials of a particular functionality in terms of configurational parameters and design new variants to enhance the functionality. This concept has been useful in extending the frontier of functional materials and successfully applied to HTSC copper oxides: most of them have been grouped into two types of "Homologous Series". Synthesis of the designed "novel material" is another major task in new material research. For the case of copper oxides, most of new members have been realized through ultra-high pressure techniques (since 1993) and filled blanks for possible members. Similar approaches have been applied to other functional materials including high-efficiency oxide thermoelectrics.

3:00 PM
Order and Stability of III-V Semiconductor Surface Alloys at Finite Temperature: *John Thomas*[1]; Joanna Mirecki-Millunchick[1]; Normand Modine[2]; Anton Van der Ven[1]; [1]University of Michigan; [2]Sandia National Laboratories

The surface structure and composition of III-V semiconductor alloys is of significant importance given the epitaxial synthesis of these materials. We develop a cluster expansion for the coupled substitutional and adsorption/desorption sublattices and apply it, via Monte Carlo, to the As-rich (2×4) reconstructed surface of $In_xGa_{1-x}As$/GaAs (001) in order to understand the effects of atomic size mismatch and temperature on surface ordering and stability. We analyze the smooth a2(2×4)-ß2(2×4) transition and directly examine the entropy and cation site occupancy in both reconstructions. There exists a strong tendency for compositionally-dependent dimer ordering in a2(2×4) as well as a chemical potential region of stability for a hybrid a2(2×4)-ß2(2×4) reconstruction, which drives pronounced composition modulation of surface cation sites. Additionally, we describe new techniques for the prediction of unknown surface structure in III-V compounds and similar systems, with results from a number of binary III-V compounds.

3:20 PM
Stability, Surface Energy and Specific Properties of Al-Based Complex Intermetallics: Esther Belin-Ferré[1]; Jean Marie Dubois[1]; [1]CNRS Institut Jean Lamour

The stability of Al-based quasicrystals, related complex and simpler compounds depends basically upon Al sp- transition element d hybridization at EF[1]. The electronic structure of bulk specimens drives wetting by water of their surfaces [2]. Electronic structure is investigated using soft X-ray emission spectroscopy that provides partial and local densities of states (DOS) in a compound. From measurements of friction coefficients in vacuum against hard steel for Al-based conventional and complex crystals and quasicrystalline icosahedral Al-Cu-Fe [3] we suggested the DOS at EF is the essential parameter determining friction and solid-solid adhesion in vacuum. Here, we report on DOS and friction measurements for binary Al-TM complex intermetallics focusing at the contribution of d states at EF. 1. E. Belin-Ferré, J. Phys.: Cond. Matter 14 R789 (2002). 2. J.M. Dubois, J. Non Cryst. Sol., 334&335 481 (2004). 3. E. Belin-Ferré and J.M. Dubois, Int. J. Mat. Res. 97 985 (2006).

3:40 PM Break

4:10 PM Invited
Simulating Atomic-Scale Phenomena with Colloids: *Frans Spaepen*[1]; [1]Harvard School of Engineering and Applied Sciences

Colloids consist of micrometer-size particles in a fluid that interact by central potentials (hard sphere or electrostatic). At large packing fractions they form phases similar to those formed by atoms in condensed matter: liquids, crystals and glasses. Since the colloidal particles are large and slow, they can be tracked in time and in three-dimensional space by confocal microscopy. Colloidal systems, therefore, are highly efficient "analog computers" for the study of the dynamics of complex multiparticle phenomena in condensed matter. A number of examples are presented: crystal nucleation, coherency dislocations in epitaxial growth, indentation of single crystals, and plastic shear of glasses.

4:40 PM Invited
Molecular Dynamics Simulations of Crystallization in Metallic Glasses: *Diana Farkas*[1]; [1]Virginia Tech

Model metallic glasses were studied using molecular dynamics simulations, creating them by fast quenching from the liquid temperature range. This talk will present the results of structure relaxation at various temperatures and the response of the glasses to applied strain. The results show that crystallization can be induced by the applied strain. The details of the atomic level configurational changes leading to the crystallization transformation will be discussed.

5:10 PM
Structure in Liquid Alloys Investigated by First-Principles Molecular Dynamics Simulations: *Mark Asta*[1]; Haxhimali Tomorr[2]; [1]University of California, Davis; [2]Northwestern University

Throughout his career Professor de Fontaine has made major contributions to the modeling and theoretical understanding of the origins and consequences of configurational short-range order (SRO) in alloy solid solutions. Just as SRO is an important feature of alloy solid solutions, local topological and chemical order in liquid alloys can have important consequences for a number of technologically important processes including crystal nucleation and growth. In this talk we review the insights into liquid alloy structure and dynamics that can be derived within the framework of first-principles molecular-dynamics simulations. We focus on applications to molten Au-Si and Au-Ge alloys, which have received considerable recent interest due to their widespread use as catalysts for semiconductor nanowire growth by the vapor-liquid-solid mechanism. We present results elucidating the nature of the liquid structure and dynamics based on calculated radial distribution functions, bond-angle distributions, common-neighbor analysis, and mean-square displacements.

5:30 PM
Quantum Mechanical Corrections to Simulated Shock Hugoniot Temperatures: *Nir Goldman*[1]; Evan Reed[1]; Larry Fried[1]; [1]Lawrence Livermore National Laboratory

We present a straightforward method for the inclusion of quantum nuclear vibrational effects in molecular dynamics calculations of shock Hugoniot temperatures. Using a Grüneisen equation of state and a quasi-harmonicapproximation to the vibrational energies, we derive a simple, post-processing method for calculation of the quantum corrected Hugoniot temperatures. We have used our novel technique on *ab initio* simulations of both shock compressed water and methane. Our results indicate significantly closer agreement with all available experimental temperature data for these two systems. Our formalism and technique can be easily applied to a number of different shock compressed molecular liquids or solids, and has the potential to decrease the large uncertainties inherent in many experimental Hugoniot temperature measurements of these systems.

Jim Evans Honorary Symposium: Electrochemical Phenomena

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division, TMS Light Metals Division
Program Organizers: Ben Li, University of Michigan; Brian G. Thomas, University of Illinois at Urbana-Champaign; Lifeng Zhang, Missouri University of Science and Technology; Fiona Doyle, University of California, Berkeley; Andrew Campbell, WorleyParsons

Wednesday PM Room: 619
February 17, 2010 Location: Washington State Convention Center

Session Chair: Fiona Doyle, University of California, Berkeley

2:00 PM Introductory Comments

2:10 PM
The Application of Electrochemical Techniques to Elucidate the Mechanisms of Copper Chemical Mechanical Planarization (CMP): *Fiona Doyle*[1]; Serdar Aksu[2]; Ling Wang[3]; Shantanu Tripathi[4]; Seungchoun Choi[1]; [1]University of California, Berkeley; [2]Solopower, Inc.; [3]Applied Materials; [4]Intel

Chemical mechanical planarization (CMP) is an important unit process in the manufacture of integrated circuits. During CMP of copper metallization lines, electrochemical oxidation phenomena act synergistically with mechanical abrasion to remove copper preferentially from protruding topography. In order to be able to optimize CMP processes, minimize defects, and model the material removal rate for process control, it is desirable to understand the mechanisms at play. Here we discuss various electrochemical studies that we have been used for this purpose, including potentiodynamic tests, in-situ polarization studies, electrochemical quartz crystal microbalance tests, and measurement of passivation kinetics using scratch-repassivation and potential-step chronomamperometry. Electrochemical impedance spectroscopy was used in the latter to distinguish capacitive charging from passivation currents. The mechanisms elucidated by these techniques are discussed, along with a mechanistic tribo-chemical model proposed for CMP.

2:35 PM
Development of Inert Anodes for Electrowinning in Calcium Chloride – Calcium Oxide Melts: Shuqiang Jiao[1]; *Derek Fray*[1]; [1]University of Cambridge

There is a need to develop inert anodes for use in calcium chloride-calcium oxide melts. Most metallic alloys severely corrode in the these melts and oxide based materials form stable insulating calcium compounds. Anodes could be made from these materials, provided the electronic conductivity can be increased. In the case of calcium titanate, there have been several attempts at doping with lower valent oxides but the increases in electronic conductivity were minor. In this work, a different approach has been adopted which was to form a solid solution with a compound that has an identical structure but is an excellent electronic conductor. Calcium ruthenate is such a compound with a room temperature conductivity of about 1000 ohm-1 cm-1. Solid solutions of calcium ruthenate and calcium titanate were found to act as anodes in calcium chloride-calcium oxide melts, evolving oxygen for over 150 hours with negligible attack.

3:00 PM
Electrochemical Characterization of Nanoparticle Silver Based Zn-AgO Batteries: *Abhinav Gaikwad*[1]; Josh Gallaway[1]; Dan Steingart[1]; [1]City College of New York

We examine the use of a nanoparticle silver ink as the basis for alkaline battery electrodes. This ink is intended as bussing material for printed electronic circuits, and despite organic additives, provides expected performance from silver with respect to electrochemical characterization. As the negative electrode in a ZnO-KOH electrolyte, it serves as a substrate for plating zinc, and as a positive electrode, it undergoes the Ag -> Ag2O -> AgO reaction. The electrochemical behavior and mechanical strength of this material will be characterized within microfluidic channels. Cell configurations and example applications will also be discussed.

3:25 PM

Molten Oxide Electrolysis for Lunar Oxygen Generation Using *in situ* Resources: Alex Vai[1]; *James Yurko*[2]; D. H. Wang[3]; Donald Sadoway[1]; [1]Massachusetts Institute of Technology; [2]Electrolytic Research Corporation; [3]22Ti LLC

Molten oxide electrolysis (MOE) is a demonstrated laboratory-scale process for producing oxygen from JSC-1A and other lunar simulants and is being pursued by NASA as a candidate process for lunar oxygen production using *in situ* resources. As part of an investigation to improve the technological readiness of critical subsystems, the technical feasibility of MOE has been studied in a laboratory-scale cell. Under constant current chronopotentiometric conditions, scaleable iridium and iridium-alloy anodes demonstrated a capability for generating more than 1 L of oxygen from a silicate melt at temperatures near 1575°C, drawing current at levels as high as 12A. Cell voltage, gas flow, and gas chromatography data will be shown from the electrolysis experiments. Real-time visual observation of the electrolysis process as well as SEM and EDX characterization of the electrodes and reaction products will be shown. Scale-up considerations for larger size reactors and future work will be discussed.

3:50 PM Break

4:05 PM

Leaching of Metal Components from Waste PCBs by Electro-Generated Chlorine in Hydrochloric Acid Solution: Eun-young Kim[1]; Min-seuk Kim[1]; *Jae-chun Lee*[1]; Kyoungkeun Yoo[1]; Manoj Kumar[1]; [1]Korea Institute of Geoscience and Mineral Resources (KIGAM)

The leaching behavior of metal components from waste printed circuit boards (PCBs) has been investigated using electro-generated chlorine in hydrochloric acid solution. The experiments were carried out by employing two different reactors: (a) a single reactor facilitated with simultaneous Cl2 generation and metals leaching, (b) a separate metal leaching reactor connected with the anode compartment of Cl2 generation. Various parameters, viz. current density, chloride concentration, leaching temperature and time, agitation speed have been studied to understand the mechanism of copper leaching using both reactors. Also, two different reactors were compared in terms of leaching efficiency for the application to the recycling of valuable metals from PCBs through hydrometallurgical route.

4:30 PM

Morphology of Zinc Studied under Additive Control within Microfluidic Channels: *Joshua Gallaway*[1]; Abhinav Gaikwad[1]; Dan Steingart[1]; [1]City College of New York

The morphology of electrodeposited metal is critical in situations where demanding physical or electrical properties of the resultant metal are required, such as with energy storage in rechargeable battery electrodes, semiconductor patterning, or metal finishing. Morphology is typically controlled by the presence of additives at ppm concentrations, which either alter the deposition mechanism or hinder troublesome side-reactions. Microfludic electrochemical cells allow quantitative observation of the effect of additives, through rapid in situ introduction or removal of the additives under plating conditions. In situ monitoring of the electrode surface and current-potential responses reveals real-time electrochemical events in a fashion impossible to achieve in, for example, a typical rotating disk electrode configuration. Millisecond resolution of such transitions allows one to observe time scales of the relevant processes, such as additive adsorption, desorption, or bubble generation. Additionally, the technique requires only small analyte volumes, and provides well-defined hydrodynamics for system modeling and analysis.

4:55 PM

Direct Write Dispenser Printed Energy Storage Devices: *Christine Ho*[1]; Jay Keist[1]; Ba Quan[1]; Paul Wright[1]; James Evans[1]; [1]University of California, Berkeley

As electronic devices become smaller in volume and more specialized in functionality, a paradigm shift in energy storage design and manufacture is beginning to emerge and can be realized with the development of simple, low-cost, solutions-based processing methods to incorporate custom energy buffers directly onto a device. We have been developing the materials and direct write fabrication methods for printing carbon based electrochemical capacitors and zinc batteries directly onto a substrate. Our materials efforts include the optimization of mechanical and ionic transport properties of ionic liquid gel electrolytes, and this has enabled the fabrication of completely printable “solid-state” capacitors and batteries, mitigating manufacturing and packaging concerns. Through a pneumatic dispenser printing system, the energy storage devices can be patterned and integrated directly on-chip. We will also present comprehensive device characterization, including long-term cycling performance and rate behavior.

Jim Evans Honorary Symposium: Modeling

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division, TMS Light Metals Division
Program Organizers: Ben Li, University of Michigan; Brian G. Thomas, University of Illinois at Urbana-Champaign; Lifeng Zhang, Missouri University of Science and Technology; Fiona Doyle, University of California, Berkeley; Andrew Campbell, WorleyParsons

Wednesday PM Room: 620
February 17, 2010 Location: Washington State Convention Center

Session Chair: Lifeng Zhang, Missouri University of Science and Technology

2:00 PM Introductory Comments

2:10 PM

Mathematical Modeling of Spooling/Unspooling Stresses in Electricity Distribution Cables: James Evans[1]; *W. Kinzy Jones, Jr*[2]; [1]UC, Berkeley; [2]Amoeba Technologies

Much of the nation’s electric power is distributed through underground cables having a central conductor carrying electricity at approximately 12,000 volts. The insulation between the conductor and the ground is only a few millimeters thick and its failure results in expensive cable replacement or occasionally an explosive event injuring, or even killing, passers-by. The insulation is subjected to electromagnetic forces that have been modeled at Berkeley but it is also subject to stresses arising prior to installation in the ground because it is wound on a spool at manufacture and subsequently unwound in the field at placement in service. The paper reports on a finite element analysis, based on measurements of the mechanical properties of the insulation, of stresses that could result in this way and that could contribute to the ultimate failure of the cable.

2:35 PM

Computational Modeling of Heap Leaching Processes: *Mark Cross*[1]; Chris Bennett[1]; Diane McBride[1]; A. Hernandez[2]; T. N. Croft[1]; J.E. Gebhardt[2]; [1]Swansea University; [2]Process Engineering Resources Inc

Heap leaching is becoming increasingly popular for the extraction of low grade ores, where copper sulphides and gold/silver/copper complexes are the most common applications, although there are others (e.g. for nickel sulphides). Although the leaching process is simple in concept, it involves what may be characterised as multi-phase reactive thermo-fluid flows in porous media. Hence, the computational modelling of this process in its industrial context is very challenging. It is worth addressing though, because model based simulation tools offer the potential for process optimisation and overall control at a level not conventionally aspired to on plants. In this paper an overview of the work done by the team over a decade is described in the development, validation and industrial deployment of heap leach models for the analysis, simulation and strategic control of plants processing both copper sulphides and gold/silver/copper oxides.

3:00 PM

A T-Ψ Potential Formulation for Numerical Simulation of Induction Heating Processes: *Nagy El-Kaddah*[1]; Thinium Natarajan[2]; [1]The University of Alabama; [2]United States Steel Corporation

This paper describes an efficient computational method for 3-D numerical simulation of induction heating processes. It is based on hybrid differential-integral formulation of the current vector potential (T) and reduced magnetic scalar potential (Ψ) of the electromagnetic field. This hybrid formulation confines the solution domain of the open boundary electromagnetic field problem to the metal, and permits full coupling of electromagnetic and heat transfer aspects of the induction heating process. The governing electromagnetic and heat transfer equations were solved using finite element method. The versatility of the developed algorithm for handling complex geometries and coil configurations is demonstrated by presenting results of numerical simulation of transverse flux induction heating (TFIH) of steel sheets during rolling.

3:25 PM
Modeling on the Cast Start during Steel Continuous Casting Process: *Yufeng Wang*[1]; Lifeng Zhang[1]; [1]Missouri University of Science and Technology

Serious defects, such as surface longitudinal cracking, inner impurities are frequently found in slabs at the beginning of the first heat casting. During this stage, molten steel is continuously filled into a cavity surrounded by mold walls and dummy bar head. The unstable fluid flow-related phenomena, including the fluctuation of molten steel, the interaction between steel phase and air phase, are the source of quality problems and manufacture accidents. And steel products from this stage are often downgraded or rejected. In order to control the process and reduce the cost, relevant investigations are performed in the current study. A three-dimensional multiphase (gas, molten steel, and mold flux) model is developed for the continuous casting process. Volume of Fluid (VOF) Multiphase method was applied to track the interface between steel phase and air phase.

3:50 PM Break

4:05 PM
Improved Computational Modeling of the Flame Spray Pyrolysis Process for Silica Nanopowder Synthesis: Miguel Olivas-Martinez[1]; *Hong Yong Sohn*[1]; Hee Dong Jang[2]; Terry Ring[1]; [1]University of Utah; [2]Korea Institute of Geoscience and Mineral Resources (KIGAM)

A computational fluid dynamics (CFD) model is presented that couples the fluid dynamics with various processes involving precursor droplets and product particles during the flame spray pyrolysis (FSP) synthesis of silica nanopowder from volatile precursors. The gas-phase processes are modeled by the governing turbulent equations of overall continuity, momentum, energy, and species mass transport. The transport and evaporation of binary liquid droplets are simulated from the Lagrangian viewpoint. The kinetics of particle formation by homogeneous nucleation and growth by Brownian coagulation are accounted for by the population balance. The latter is solved by the quadrature method of moments (QMOM), which makes no prior assumption on the particle size distribution (PSD). Results for the simulation of silica nanopowder synthesis by the gas-phase thermal oxidation of tetraethylorthosilicate in a bench-scale FSP reactor are presented. The effects of the feed rates of dispersion air and precursor solution on the PSD have been evaluated.

4:30 PM
Global and Local Stability of Magnetically-Levitated Droplets: *Ben Li*[1]; X. Ai[1]; Y. Huo[1]; [1]University of Michigan

This paper presents a numerical study of the global stability of and the local linear and nonlinear magnetically-induced flow instability in a liquid droplet levitated in an alternating magnetic field. The numerical solution of the full 3-D, time harmonic Maxwell equations is obtained using the combined finite element and boundary element method. The computational model, validated for a microwave processing system, is then used to predict the asymmetric electromagnetic forces induced by the induction coils in a liquid droplet. Its global stability and the accompanying temperature distribution are studied using model for various perturbed configurations. The linear and nonlinear flow stabilities of the magnetically-levitated droplet are studied based on the high-order finite difference solution of the Navier-Stokes equations with induced electromagnetic forces. Both linear and nonlinear phenomena are studied and the numerical results are compared with experimental observations.

4:55 PM
Dynamics of Magnetically Levitated Liquid Droplets: Valdis Bojarevics[1]; *Koulis Pericleous*[1]; Alan Roy[1]; Stuart Easter[1]; [1]University of Greenwich

A number of different methods have been developed, which allow the noncontact electromagnetic levitation of liquid metal droplets to investigate the melting/solidification process and measure the properties of these highly reactive materials. The intense AC magnetic field required to produce levitation in terrestrial conditions, along with the buoyancy and thermo-capillary forces, results in turbulent convective flow within the droplet. The presented numerical results show that the use of a homogenous DC magnetic field allows the large scale flow to be damped. However the turbulence properties are affected at the same time, leading to a lower turbulent damping. The reduction in the AC field driven flow in the main body of the drop leads to a noticeable thermo-capillary convection at the edge of the droplet, thus affecting the thermal loss and solidification. An alternative method without internal electric currents, using high gradient D.C. magnetic levitation, is analyzed analytically and numerically.

5:20 PM
Mangetically-Damped Flows: Numerical Simulations and Experimental Measurements: *Ben Li*[1]; X. Bing[1]; Y. Shu[1]; [1]University of Michigan

This paper presents a study on magnetic damping of metal flows with and without the effect of gravity. Comprehensive numerical models are developed for the purpose of simulating electromagnetic and transport phenomena in the media with and without radiative transfer participating. The numerical models are based on the combined continuous and discontinuous finite element solution of the Maxwell equations, radiative transfer equations, Navier-Stocks equations and energy balance equations.Accompany experimental measuring systems were developed where SCN and liquid gallium are used as simulating liquid. Flow measurements were taken by particle velocimetry and hot wire probes for certain configurations. The measurements are compared with the numerical models. With validated models, extensive numerical simulations are conducted to study the magnetic-damping phenomena in various flow figurations for applications in space materials processing applications.

Magnesium Technology 2010: Effects of Heat Treatment and Casting Process

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Magnesium Committee
Program Organizers: Sean Agnew, University of Virginia; Eric Nyberg, Pacific Northwest National Laboratory; Wim Sillekens, TNO; Neale Neelameggham, US Magnesium LLC

Wednesday PM — Room: 613
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Elhachmi Essadiqi, CANMET ; Zi-Kui Liu, The Pennsylvania State University

2:00 PM
On Mechanical Properties and Microstructures of TTMP Wrought Mg Alloys: Jack Huang[1]; Tamir Arbel[2]; Laura Ligeski[2]; Jesse McCaffrey[1]; Sanjay Kulkarni[1]; J. Jones[2]; Tresa Pollock[2]; *Raymond Decker*[1]; Steve LeBeau[1]; [1]Thixomat; [2]University of Michigan

Thixomat has recently developed a simplistic innovative process for producing high strength wrought Mg sheet cost effectively, the T (Thixomolding) TMP (Thermomechanical Processing) process. The theoretical basis behind this TTMP process is by leveraging the inherent fast cooling nature of the Thixomolding process to produce fine-grained starting sheet stock for the enablement of the high-strain thermomechanical forming step. Recent mechanical property characterization of the TTMP wrought sheets consistently shows tensile yield strength of 300MPa, ultimate tensile strength of 350MPa, and elongation at break of 10% or higher. To further understand the correlation between the enhanced resultant mechanical properties and the deformation mechanism(s) as well as the microstructures of the wrought sheet, we set out to characterize, via microscopic and x-ray diffraction techniques, the grain structures at various stages of the TTMP process. Observations on probable correlation between enhancement of the mechanical properties and microscopic/mechanistic features will be reported.

2:20 PM
The Effect of Thermomechanical Processing on the Tensile and Fatigue Behavior of Thixomolded® AM60: *Zhe Chen*[1]; B. Kuhr[1]; Alex Ritter[1]; Jack Huang[2]; Ray Decker[2]; Steve LeBeau[2]; Carl Boehlert[1]; [1]Michigan State University; [2]Thixomat

Tensile and fatigue experiments were performed at RT and 150°C on AM60 after three processing treatments: (1) as-thixomolded (as-molded), (2) Thixomolded then thermo mechanically processed (TTMP) and (3) TTMP then annealed (annealed). The TTMP procedure resulted in a significantly reduced grain size and a tensile strength greater than twice that of the as-molded material without a debit in elongation-to-failure. The as-molded material exhibited the lowest strength while the annealed material exhibited an intermediate strength but the highest elongation-to-failure (>17%). The as-molded material exhibited the lowest fatigue threshold values and the lowest fatigue resistance. The annealed material exhibited the greatest fatigue resistance and this was suggested to be related to its balance of tensile strength and ductility. Overall the results indicate that TTMP processing of AM60 dramatically improves the mechanical behavior making this alloy attractive for structural applications in the automotive, aerospace, wind energy, and biomedical industries.

2:40 PM
Influence of the Heat Treatment on Mechanical Properties and Microstructure in LPSO Mg-Zn-Y Alloys: *Masafumi Noda*[1]; Tyuyoshi Mayama[1]; Yoshihito Kawamura[1]; [1]Department of Materials Science, Kumamoto University

Mg−Zn−Y alloys are composed of α−Mg and LPSO phases. The extruded Mg−Zn−Y alloys are known to have dramatically enhanced strength because the kink deformation occurring in the LPSO phase during plastic deformation. In this present study, the effect of heat treatment on mechanical properties and the thermal stability of microstructure in Mg−Zn−Y extruded alloys were investigated. The elongation of the alloys achieved to about twice while its high strength was retained up to heat treatment temperature of 623 K with no change in the microstructure compared with extruded alloys. On the other hands, yield stress and tensile strength decreases while elongation improves in 623K or more so that α−Mg phase grain growth. Even at heat treatment temperature of 623 K, it was possible to maintain high strength and thermal stable structure.

3:00 PM
The Effect of Zn Additions on Precipitation Hardening of Mg-Ca Alloys: *Brian Langelier*[1]; Shahrzad Esmaeili[1]; [1]University of Waterloo

Precipitation hardening can be an effective mechanism for enhancing the strength of magnesium alloys. Calcium is known to provide grain refinement and creep resistance to magnesium casting alloys, and may also be utilized for precipitation hardening through formation of the Mg2Ca phase. The hardening effect in binary Mg-Ca alloys is small, but may be significantly improved by the addition of Zn. The effect of Zn on the precipitation hardening behavior of Mg-Ca-(Zn) alloys is characterized with combined differential scanning calorimetry and microhardness measurements, as well as FactSage thermodynamic analysis. Zn additions result in the precipitation of ternary phases, and the refinement of precipitates. Precipitate refinement is attributed to an altered precipitation sequence in the Mg-Ca-Zn alloys. The results of this work show the effectiveness of combined thermal-mechanical and thermodynamic analysis in characterizing the effects of alloying element additions on precipitation hardening in magnesium.

3:20 PM
The Recent Developments in Mg-Sn Based Alloy Thermodynamic Database: *Manas Paliwal*[1]; Jina Kim[1]; Daehoon Kang[1]; In-Ho Jung[1]; [1]McGill University

Mg-Sn based alloy is one of the most promising Mg alloys for high temperature applications. In order to keep pace with the Mg-Sn alloy development, the Mg-Sn based alloy database has been developed for many years. Thermodynamic calculations based on the accurate thermodynamic database can provide invaluable information for the alloy design such as liquidus/solidus temperature, secondary phase precipitation, heat treatment temperature, etc. In the present study, the recent thermodynamic optimizations for the Mg-Sn-Ca, Mg-Ge-Si, Mg-Ge-Sn, Mg-Pb-Si, Mg-Pb-Sn, Mg-Al-Bi and Mg-Al-Sb ternary systems will be presented. In addition, the applications of the updated thermodynamic database to new Mg-Sn alloy design will be presented.

3:40 PM Break

4:00 PM
Influence of Zn Additions on Age Hardening Response and Microstructure of Mg-0.3at.%Ca Alloys: *Keiichiro Oh-ishi*[1]; Chamini Mendis[1]; Ryuichi Watanabe[2]; Kazuhiro Hono[1]; [1]National Institute for Materials Science; [2]Graduate School, University of Tsukuba

The age-hardening response of creep-resistant Mg-Ca alloys has been known to be improved by the trace addition of Zn. We have investigated the age hardening responses and corresponding microstructures of Mg-0.3Ca-xZn (x = 0.0, 0.1, 0.3, 0.6, 1.0, 1.6 at.%) alloys by hardness test, transmission electron microscopy (TEM), and high-angle annular dark field-scanning transmission electron microscopy (HAADF-STEM). Zn additions up to x = 0.6 lead to enhanced age hardening responses with the highest peak hardness of Hv = 69 for x = 0.6. Further addition of Zn degraded the age hardening responses. The peak aged Mg-0.3Ca-0.6Zn alloy showed finer precipitates than the binary Mg-0.3Ca alloy. HAADF-STEM images revealed that the finely dispersed monolayer G.P. zones with internal ordered structure are the major contributor to the age hardening. Excess addition of Zn resulted in the formation of Ca2Mg6Zn3 precipitates suppressing the formation of the ordered G.P. zones.

4:20 PM
Effect of Aging and Thermomechanical Processes in Twin Roll Cast Mg AZ91 Alloy Sheet: *Ozgur Duygulu*[1]; Selda Ucuncuoglu[1]; Gizem Oktay[1]; Onuralp Yucel[2]; Ali Arslan Kaya[3]; [1]TUBITAK Marmara Research Center; [2]Istanbul Technical University; [3]Mugla University

6 mm thick and 1500 mm wide magnesium alloy AZ91 sheet was produced by twin roll casting. Sheets were homogenized between 350-475°C for 1-24 h. Afterwards, they were hot rolled down to 1 mm. Age hardening was also performed on twin roll cast AZ91 alloy sheets. Specimens were aged at 100-300°C for up to 100 h. Characterization was performed by light microscope, SEM-EDS, TEM-EDS, EPMA and XRD after twin roll casting and also after each thermomechanical process including aging. Tensile tests were performed for mechanical properties. Moreover, the age-hardening response of Mg AZ91 alloy was examined by micro hardness test.

4:40 PM
Experimental Studies on the As-Cast Microstructure of Mg-Al Binary Alloys with Various Solidification Rates and Compositions: *Dae Hoon Kang*[1]; Manas Paliwal[1]; Elhachmi Essadiqi[2]; In-Ho Jung[1]; [1]McGill University; [2]CANMET-MTL

As the solidification rate is undoubtedly the most important processing parameter to determine the as-cast microstructure and consequent mechanical properties of alloys, there have been many approaches to clarify qualitatively the effect of solidification rate on segregation and microstructural features. In the present study, the Mg-Al alloys of 3, 6 and 9 wt% Al were cast with different cooling rates, and their as-cast microstructures were examined to determine the influence of cooling rate on the segregation fraction and compositional variation. In addition, a simple kinetic solidification model associated with the thermodynamic database was developed to simulate the as-cast microstructures of Mg-Al alloys.

5:00 PM
Impurity and Tracer Diffusion Studies of Magnesium and Its Alloys: Sarah Brennan[1]; Andrew Warren[1]; Kevin Coffey[1]; *Yongho Sohn*[1]; Nagraj Kulkarni[2]; Peter Todd[3]; [1]University of Central Florida; [2]University of Tennessee; [3]Oak Ridge National Laboratory

An Integrated Computational Materials Engineering (ICME) approach for optimizing processing routes for Mg-alloys requires reliable thermodynamic and diffusion databases. We are developing a tracer diffusion database using both stable and unstable isotopes for Mg-alloys. Mg and Zn tracer diffusion studies in several polycrystalline Mg-Al-Zn alloys were conducted using the thin film method. Approximately 500 nm thick Mg, and Zn enriched isotopic films were deposited on in-situ RF plasma-cleaned polycrystalline Mg-alloys by DC magnetron sputtering from pure targets. Specimens were then diffusion annealed at various temperatures below 600°C in quartz capsules that were evacuated to 10-8 torr and backfilled with Ar-H2 mixtures. Concentration profile of Mg and Zn isotopic diffusion profiles into single phase Mg-Al-Zn alloys was determined by depth-profiling technique using secondary ion mass spectroscopy. The Mg and Zn tracer diffusion coefficients determined as a function of temperature and composition for the various Mg-Al-Zn alloys will be presented and discussed.

5:20 PM
Effect of Alloying and Solidification Rates on Microstructure of Hot Rolled and Annealed Micro-Alloyed Az31 Sheet: *Elhachmi Essadiqi*[1]; Amjad Javaid[2]; Mahmoud Shehata[2]; Teddy Muller[3]; Stephene Yue[4]; Ravi Verma[5]; [1]CANMET ; [2]CANMET; [3]Evry University; [4]McGill University; [5]General Motors

A possible process to produce Mg strip using twin roll casting begins with 3 to 10 mm thick Mg alloys strip that will be hot rolled to sheet with low cost for automotive application. To optimize the as-cast strip thickness, there is a need to determine the minimum hot rolling reduction of these strips required to produce 1 to 2 mm thick sheet with targeted properties. In this study, as-cast micro-alloyed AZ31 plates with different thicknesses (6 to 18 mm) have been rolled to 1.5 mm thick sheets and annealed. The influence of the as-cast microstructures and micro-alloying on the final hot rolled and annealed microstructure and mechanical properties has been established. The optimum hot rolling reduction required to produce targeted properties has been determined

5:40 PM
Texture and Anistropy of Continuous Cast (CC) and Direct Chill Cast (DC) AZ31 Magnesium Sheets: Raj Mishra[1]; *Jon Carter*[1]; Sooho Kim[2]; [1]GM R&D; [2]GM R&D (retired)

This study compares the microstructure and mechanical properties of CC and DC AZ31 sheets. In O-temper, the grain sizes are homogeneous through the sheet thickness, but the CC sheet has a slightly finer grain size. The c-axes of grains lie normal to the sheet surface with the prism planes distributed nearly randomly. The tensile yield strength values are nearly the same in both materials in the rolling direction (RD) and increase from RD to TD (transverse direction). The flow curves are asymmetric on the sheet plane with YS in compression being ~40% less than that in tension. The ultimate tensile strengths are independent of in-plane orientation and elongation of CC sheet decreases from RD to TD. The compression data in the sheet normal direction (ND) is similar to the tensile data in the RD or TD, but the compression data in RD shows an S-shape, characteristic of twinning.

Materials in Clean Power Systems V: Clean Coal-, Hydrogen Based-Technologies, Fuel Cells, and Materials for Energy Storage: SOFC, PEM and DMFC

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS Structural Materials Division, TMS/ASM: Corrosion and Environmental Effects Committee, TMS: Energy Conversion and Storage Committee
Program Organizers: Xingbo Liu, West Virginia University; Zhenguo Yang, Pacific Northwest National Lab; K. Weil, Pacific Northwest National Lab; Mike Brady, Oak Ridge National Lab; Jay Whitacre, Carnegie Mellon University; Ayyakkannu Manivannan, National Energy Technology Laboratory; Zi-Kui Liu, Penn State University

Wednesday PM Room: 211
February 17, 2010 Location: Washington State Convention Center

Session Chairs: K. Scott Weil, Pacific Northwest National Lab; Rod Borup, Los Alamos National Laboratory

2:00 PM
Kinetics of Oxide Scale Formation on Nicrofer-6025HT at Elevated Temperatures for Advanced Coal Based Power Plants: *Vineet Joshi*[1]; Alan Meier[1]; Scott K. Weil[2]; Jens T. Darsell[2]; [1]Alfred University; [2]Pacific Northwest National Laboratories

Oxygen separation membranes for clean coal energy delivery in advanced coal based power plants rely on use of solid state mixed ionic/electronic conductors which operate at temperatures in the range 700-900°C. Nicrofer-6025HT is a nickel based alloy which shows compatibility with these systems. Nicrofer has been proposed as a manifold material to transport the hot gases into these oxygen separation membranes. The present work investigates the kinetics of oxide scale formation on Nicrofer. Electron dispersive spectroscopy, wavelength dispersive spectroscopy and X-Ray photoelectron spectroscopy were used to characterize the oxide scale. It was observed that the oxide scale consisted primarily of two layers, an outer scale of chromium oxide and an alumina scale beneath it.

2:20 PM
Electrochemical Characterizations of Ni-YSZ Electrode in the Thin NiFe Supported Solid Oxide Fuel Cell: *Kyeong Hyun Kim*[1]; Young Min Park[2]; Haekyoung Kim[1]; [1]Yeung Nam University; [2]Research Institute of Industrial Science and Technology

Metal-supported solid oxide fuel cells (SOFCs) have been discussed as a next generation SOFC configuration due to good mechanical properties and thermal shock resistance. NiFe alloy is one of the most promising metallic materials as a supporter because of similar thermal expansion coefficient with the ceramic electrolyte. The thin NiFe supported SOFC, NiFe/Ni-YSZ/YSZ/LSCF, have been successively fabricated through tape casting and co-firing method. In order to study the effects of morphologies and components in anode electrode, the particle size and the composition of Ni and YSZ were controlled. The electrochemical performances will be discussed in terms of the fuel utilization and temperature. The long term stability will also be presented with the electrode morphologies.

2:40 PM
Metal-Supported Solid Oxide Fuel Cell: *Gyeong Man Choi*[1]; Hyup Je Cho[1]; Young Min Park[2]; [1]POSTECH; [2]RIST

SOFC (Solid Oxide Fuel Cell) has advantages in efficiency, power density, life time and multifuel capability. However, SOFC is very weak against mechanical or thermal shock due to its inherent brittleness and the low thermal conductivity of the component materials. SOFC is commonly manufactured either in the form of electrolyte-supported or anode-supported type. However, metal-supported SOFC is more promising due to its mechanical strength, thermal shock resistance, and low cost etc.. The high mechanical and thermal strength of the supporting metal compensates the weakness of ceramics and thus strengthens the cell. In this study, we have developed a thin (<~250 μm) metal-supported SOFC using a simple and common co-sintering process. The strong and thin structure gives flexible nature to SOFC. In the presentation, we will discuss the fabrication technique and electrochemical performance. The performance is comparable to or better than the conventional electrolyte- or anode-supported SOFC.

3:00 PM Invited
Development of Niobium Coated Stainless Steels as Bipolar Plate Materials for PEMFC Stacks: *Sung-Tae Hong*[1]; K Scott Weil[2]; Yong-Zoo You[1]; [1]University of UIsan; [2]Pacific Northwest National Laboratory

Niobium (Nb) coated stainless steel (SS) is being developed as a metallic bipolar plate material for PEMFC stacks. Roll boning process has been used to fabricate Nb-clad SS. The result of prior work has shown that the Nb-clad SS is electrochemically viable, exhibiting passivating behavior with current densities that were comparable to non-corrosive noble metals such as Pt. However, during the post-roll annealing process, a brittle interfacial layer may form between the two bonded materials. The brittle interfacial layer may act as an additional design constraint in forming of bipolar plates. Recently, as an alternative of roll bonding process, sputtering has been used to fabricate Nb-sputtered SS as bipolar plate materials for PEMFC stacks. The experimental result shows that the electrochemical properties of the Nb-sputtered SS can be compatible with those of the Nb-clad SS while keeping the thickness of Nb layer a few times thinner than Nb-clad SS.

3:40 PM Break

3:50 PM Invited
PEM Fuel Cell Material Durability and Degradation: *Rod Borup*[1]; Rangachary Mukundan[1]; John Davey[1]; David Wood[1]; [1]Los Alamos National Laboratory

The durability of polymer electrolyte membrane (PEM) fuel cells is a major barrier to the commercialization for transportation and stationary power applications. Each component and material in the fuel cell has different characteristics, different operational considerations and potentially different durability concerns. Within a PEMFC, the individual components are exposed to an aggressive combination of strong oxidizing conditions, liquid water, strongly acidic conditions, high temperature, high electrochemical potentials, reactive intermediate reaction products, a chemically reducing atmosphere at the anode, high electric current, and large potential gradients. To improve durability, it is important to understand the roles of these various conditions in material degradation processes and work to improve material durability. Topics for discussion will include durability testing methods including accelerated stress testing (AST), the effect of operating conditions on durability, and focus on the various component materials: membranes, electrocatalysts, catalyst supports, gas-diffusion media and bipolar plates.

4:30 PM
Performance of Micro-DMFCs with Two Kinds of Flow Fields: *Yuhao Lu Lu*[1]; Ramana Reddy[1]; [1]The University of Alabama

Micro fuel cells have been recognized as promising electrochemical power sources in portable electronic devices due to their safety, high efficiency renewable fuel, and environmental compatibility. Although performance of a micro-DMFC depends on all its components, its behavior is drastically affected by different flow fields fabricated on the end plates. In addition, scaling effects of micro-channels make the flow fields have different performance in micro-DMFCs from in conventional DMFCs as well. This study evaluated performance of micro-DMFCs with two kinds of flow fields including single-channel and double-channel serpentine designs. Polarization, electrochemical impedance spectroscopy, and chronoamperometery were employed to obtain the electricity output, resistance, and response time of micro-DMFCs at different conditions, respectively. Results showed that micro-DMFC with double-channel serpentine flow field presented a better performance than single-channel serpentine design. Meanwhile, double-channel design also demonstrated the faster response than single design when the electric load was changed.

4:50 PM
Pre-Oxidized and Nitrided Stainless Steel Foil for Proton Exchange Membrane Fuel Cell Bipolar Plates: Michael Brady[1]; Todd Toops[1]; *Peter Tortorelli*[1]; Heli Wang[2]; John Turner[2]; Harry Meyer[1]; Karren More[1]; Fernando Garzon[3]; Tommy Rockward[3]; Don Gervasio[4]; Francisco Estevez[5]; Jim Rakowski[6]; [1]Oak Ridge National Lab; [2]National Renewable Energy Lab; [3]Los Alamos National Lab; [4]Arizona State University; [5]AGNI-GenCell; [6]ATI Allegheny Ludlum

Developmental Fe-20Cr-4V alloy and 2205 stainless steel foils were pre-oxidized and nitrided to form low-interfacial contact resistance (ICR), corrosion-resistant surfaces. Promising corrosion resistance for both materials was observed under simulated aggressive anode- and cathode-side bipolar plate conditions. Variation in ICR values were observed for treated 2205 foil, and lower (better) values generally observed for the treated Fe-20Cr-4V. Single-cell, fuel cell testing of stamped and pre-oxidized/nitrided foils was conducted with a repeating cycle of 0.6V (30 min), 0.7V (20 min), 0.5V (20 min) and open-circuit voltage (1 min) out to 1000 h. Benchmark untreated stainless steel foil and machined graphite plates also were evaluated. The pre-oxidized and nitrided Fe-20Cr-4V alloy exhibited the best performance of the examined materials. Post-test analyses of the membrane electrode assemblies (MEAs) by x-ray fluorescence indicated an Fe concentration of only 0.1-0.3 x10-6 g/cm2 in the MEAs tested with the pre-oxidized and nitrided Fe-20Cr-4V and graphite plates.

5:10 PM
Effect of Pretreatment and Surface Treatment Conditions on Corrosion Resistance Property in Metallic Bipolar Plate Materials: Kee-Do Woo[1]; *Min-seok Moon*[1]; Eui-pyo Kwon[1]; Sang-hyuk Kim[1]; Duck-soo Kang[1]; Zhiguang Liu[2]; Xiao-peng Wang[1]; [1]Chonbuk National University; [2]Harbin Institute of Technology

Fuel cell is one of the new energy systems. But fuel cell components are very expensive. Therefore, development of new process or materials for fuel cell components with reduced manufacturing cost has been becoming an important issue in fuel cell industry. The possibility of replacement of the graphite bipolar plate to metallic bipolar plate was studied. In this study, three types of stainless steel were investigated. Electrochemical property of stainless steel that can be used for metallic bipolar plate was investigated in accordance with the conditions of pre-treatment and surface treatments by using Potentiodynamic analyzer. Reaction behaviors of main elements of the stainless steels within similar PEMFC/DMFC(Proton exchange membrane fuel cells/Direct-methanol fuel cells) corrosion condition were investigated by using XRD, ICP and FE-SEM observation. In comparison, austenite base stainless steel has good potentiodynamic value. Corrosion current densities (Icorr) of STS316, STS304 and STS430 were 3.5~5.2x10-7amp/cm2, 3.8~5.1x10-7amp/cm2 and 1.9~7.4x10-6amp/cm2, respectively. Interfacial contact resistance has different behavior between As-polished and As-Received condition on the same material. Normally as-polished has good contact resistance better than as-received condition. Comparison of contact resistance on STS316, as-polished specimen has 31.125(mΩcm2) and as-received specimen has 322.925(mΩcm2) with compaction pressure approx. 120N/cm2.

Modeling, Simulation, and Theory of Nanomechanical Materials Behavior: Physics of Defects, Dislocation Nucleation and Fracture II

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS/ASM: Computational Materials Science and Engineering Committee, TMS: Nanomechanical Materials Behavior Committee
Program Organizers: Thomas Buchheit, Sandia National Laboratories; Sergey Medyanik, Washington State Univ.; Douglas Spearot, University of Arkansas; Lawerence Friedman, Penn State University; Edmund Webb, Sandia National Laboratories

Wednesday PM — Room: 304
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Harley Johnson, University of Illinois; Douglas Spearot, University of Arkansas

2:00 PM Invited
Multiple Time Scale Analysis of the Ion Bombardment Surface Instability: *Harley Johnson*[1]; Kallol Das[1]; Nagarajan Kalyanasundaram[1]; Maryam Ghazisaeidi[1]; Jonathan Freund[1]; [1]University of Illinois

Low temperature ion irradiation of materials often results in nanoscale surface topology modification, ranging from the formation of dots and parallel or perpendicular ripples, to smoothening, depending upon the incident beam angle. Using a combined atomistic and continuum simulation method, we study the origins of the surface instability that gives rise to this interesting phenomenology. Thousands of single ion impacts are first studied at different incidence angles using molecular dynamics (MD). A continuum simulation then incorporates the individual "crater functions" gathered from MD into a model that includes surface diffusion over much longer time scales. We show that local mass redistribution along the surface plays a dominant role in determining the growth rate and orientation of surface features. Finally, we introduce an alternative method for spanning the time scales in the high temperature problem, when the surface is affected not only by sputtering and surface diffusion, but also by recrystallization.

2:30 PM
Stress and Strain near Rough Surfaces and Interfaces: *Lawrence Friedman*[1]; [1]Penn State University

The importance of surface roughness is well known for strained surfaces and interfaces. Surface roughness can concentrate stress at the micro- and nano-scales; conversely, stress and strain can drive surface roughening such as in Stranski-Krastanow and Volmer-Webber growth. Similar phenomena result for internal surfaces effecting long-range stress fields as well as net interfacial energies with impacts on adhesion and delamination. Here a Green function method is used to calculate stress fields and interfacial energies to arbitrary order in surface and interface roughness. Numerical requirements and limitations are presented along with applications to the stochastic formation of self-assembled quantum dots such as Ge_xSi_{1-x}/Si and thin-film adhesion energies.

2:50 PM
Saddle-Node Scalings during Dislocation Nucleation in Perfect Crystals under Inhomogeneous Loads: *Asad Hasan*[1]; Craig Maloney[1]; [1]Carnegie Mellon University / Civil & Environmental Engineering

Under sufficiently high loads, dislocations will be nucleated in perfect crystals. An outstanding issue is the prediction of where and under what loads nucleation will occur. Many criteria have been put forward which address this question, some in terms of the local stress field, others in terms of the local tangent stiffness of the material. More recently it has been questioned whether a local criterion can be used at all [1]. We perform molecular dynamics simulations to address these questions. We show that nucleation can be understood in terms of a classical saddle-node bifurcation, during which the velocity of the system concentrates onto a single mode which couples linearly to the applied deformation. These scalings should have important implications for the estimation of the nucleation rate via classical rate theory. [1] R.E. Miller and D. Rodney, J. Mech. Phys. Solids 56 (4) 1203-1223, 2008.

3:10 PM
Phase Stability and Transformations in NiTi from Density Functional Theory Calculations: *Karthik` Guda Vishnu*[1]; Alejandro Strachan[1]; [1]Purdue University

We used density functional theory to characterize various crystalline phases of NiTi alloys: i) high temperature austenite phase B2, ii) orthorhombic B19, iii) the monoclinic martensite phase B19', and iv) a body centered orthorhombic phase (B33), theoretically predicted to be the ground state. We also investigated possible transition pathways between the various phases and the energetics involved. Interestingly, We predict a new phase of NiTi, denoted B19'', which is involved in the transition between B19' and BCO. B19'' is monoclinic and can exhibit shape memory. We find B19 to be metastable with a 4 meV energy barrier separating it from B19'. We would also like to show our large scale molecular dynamics (MD) simulation results to understand the role of size in martensitic transformation at nano scale.

3:30 PM Break

3:50 PM Invited
Coupled Continuum - Density Functional Theory Investigation of Crack-Tip Propagation and Dislocation Nucleation: Arun Nair[1]; *Derek Warner*[1]; Richard Hennig[1]; [1]Cornell University

Atomic-scale modeling of deformation processes has long been plagued by the challenge of accurately and efficiently describing the complexities of multispecies bonding. In the case of metals, this has lead to the majority of the atomistic modeling effort focusing on pure elemental metals in a vacuum, rather than more technologically relevant problems involving alloys with impurities in realistic environments. In an attempt to address this long-standing challenge we have employed a concurrent multi-scale approach that couples an atomistic region whose forces are calculated via Kohn-Sham Density Functional Theory to a continuum region described by linear elasticity. This approach enables us to examine large simulation cell sizes and thus properly account for the long-range elastic fields associated with key defects such as dislocations. This talk will specifically focus on the application of the above method to crack-tip phenomenon in aluminum in the presence of oxygen.

4:20 PM
Modeling of Magnetic Thin Film with Misfit Dislocations: *Nirand Pisutha-Arnond*[1]; Bo Yang[2]; Dong-Hee Lim[1]; Mark Asta[2]; Katsuyo Thornton[1]; [1]University of Michigan; [2]University of California, Davis

We present multiscale calculations of misfit dislocations to study dislocation energetics and structures within heteroepitaxial Fe films grown on Mo(110) and W(110) substrates. On the atomic level, we calculate the generalized stacking fault energies of the Fe/Mo and Fe/W systems from the density functional thoery, which are used as an input to the continuum models. On the continuum level, the Peierls-Nabarro formulation is employed to calculate the elastic field originating from the misfit dislocations within a film of finite thickness. The semi-analytical and numerical methods are used for planar and non planar films. By allowing the dislocation spacing to vary and by including the effect of homogeneous strain, the equilibrium dislocation spacing as a function of film thickness is obtained. We relate these results to the surface instability mechanism and the metastable height observed in the Fe/Mo and Fe/W systems.

4:40 PM
Strain Engineering on Si/Ge Nanoscale Heterostructures: *Yumi Park*[1]; Winnie Tan[1]; Alejandro Strachan[1]; [1]Purdue University

Strained heterostructures are ubiquitous in microelectronic applications and the ability to control strain is critical to improve their electronic properties. We use molecular dynamics to explore nanopatterning and local amorphization followed by re-crystallization as possible avenues for strain engineering. Nanopatterning of strained Si/Ge/Si heterostructures into 1-D bars leads to transverse strain relaxation in the Ge section due to surface relaxation and we characterize how this relaxation increases with decreasing the bar width (W) and increasing the Ge thickness (H). Local amorphization of Si/Ge nanolamintes also leads to strain relaxation in the direction normal to the crystal/amorphous interface that increases as the height of Si/Ge bi-layer (H) increases and the periodic length of the crystalline/amorphous pattern (W) decreases. In both cases, a full strain relaxation is achieved for roughly square cross section (H≈W) leading to a uniaxial strain state, which is desirable for high-speed electronics.

5:00 PM
Anomalous Dissipation in Single-Walled Carbon Nanotube Resonators: *Peter Greaney*[1]; Giovanna Lani[2]; Giancarlo Cicero[3]; Jeffrey Grossman[1]; [1]Massachusetts Institute of Technology; [2]Ecole Polytechnique; [3]Polytechnic of Torino

We observe transient anomalous dissipation during molecular dynamics simulation of the ring-down of flexural modes in single-walled carbon nanotube (CNT) resonators. During the anomalous regime the quality factor of the mode can be reduced by more than 95% for tens of picoseconds. The anomalous dissipation is sensitive to the CNT temperature and the energy in the mode, and remarkably increasing the excitation energy in the resonator causes it to decay to zero faster. This counter intuitive phenomenon is analogous to the Mpemba effect in the freezing of water, and as with the Mpemba effect, it implies that the background temperature in the system does not uniquely define its dissipative state. Using a projection algorithm we are able to follow the energy as it dissipates, identifying gateway modes that mediate the dissipation, and a resulting athermal phonon population. The implications for these observations for continuously driven resonators are discussed.

Neutron and X-Ray Studies of Advanced Materials III: Diffuse Scattering II

Sponsored by: The Minerals, Metals and Materials Society, ASM International, TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee, TMS: Titanium Committee
Program Organizers: Rozaliya Barabash, Oak Ridge National Laboratory; Jaimie Tiley, Air Force Research Laboratory; Erica Lilleodden, GKSS Research Center; Peter Liaw, University of Tennessee; Yandong Wang, Northeastern University

Wednesday PM — Room: 303
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Darren Goosens, Australian national University; Yang Ren, Argonne National Laboratory

2:00 PM Keynote
Monte Carlo Simulation of Disorder in the Ag^+ Fast Ion Conductors Pearceite and Polybasite: *Richard Welberry*[1]; [1]Research School of Chemistry

The pearceite–polybasite group of minerals (i.e. pearceite, antimonpearceite, arsenpolybasite and polybasite), of general stoichiometry $[M^{I}_{6}T^{III}_{2}S_{7}][Ag^{I}_{9}Cu^{I}S_{4}]$ with $M=Ag^+$, Cu^+ and $T=As^{3+}$, Sb^{3+}, occur relatively commonly in nature. All have recently been shown to exhibit Ag^+ fast ion conduction at rather low temperatures (only slightly above or below room temperature). The average crystal structure determination of these materials shows the positions of the Ag^+ ions to be smeared out or delocalised within sheets in an ordered framework structure comprised of the remaining ions. At the same time, strong and highly structured diffuse scattering has been observed which contains diffuse peaks that are incommensurate with the diffraction peaks of the framework structure. In order to try to understand the origins of the fast ion conduction properties of these materials we have used Monte Carlo computer simulation of a model system to interpret and analyse this observed diffuse scattering.

2:30 PM Invited
Monte Carlo Modelling of Diffuse Scattering from Single Crystals: *Darren Goossens*[1]; Aidan Heerdegen[1]; [1]Australian National University

Diffuse scattering probes the local ordering in a crystal, whereas Bragg peaks are descriptive of the average long-range ordering. The population of local configurations can be explored by modelling the three-dimensional distribution of diffuse scattering. Local configurations are not constrained by the average crystallographic symmetry so one way of modelling diffuse scattering is by modelling a disordered (short-range ordered) structure and then calculating its diffuse scattering. The structure must contain enough unit cells to give a statistically valid model of the populations of local configurations, and so requirements for a program to model this ordering are very different from programs which model average crystal structures (used to fit the Bragg diffraction). The strategies used to tackle the problem and the way in which they are implemented will be discussed.

2:50 PM Invited
Phase Transition under High Pressure in Ionic Liquid Based Mixtures: *Hiroshi Abe*[1]; Yusuke Imai[1]; Takefumi Goto[1]; Takahiro Takekiyo[1]; Yukihir Yoshimura[1]; [1]National Defense Academy

Room temperature ionic liquids (RTILs) have been big subjects of an environmentally "green" chemistry. Recently, anomalous domain growth was observed in [DEME][BF_4]-H_2O mixtures.[1] The anomaly causes superstructure and volume contractions.[2] In this study, we investigate isotope effect in hydrogen/deuterium (H_2O, DHO and D_2O) using [DEME][BF_4]-water mixtures by the simultaneous measurements. Crystallization temperature decreases by isotope effect in deuterium of water. Nucleation process in the mixture is suppressed instead of little water concentrations (≅ 1 mol%). At the same time, anomalous domain growth, superstructure and volume contractions disappear accompanied by the isotope effect of water. [1] Y. Imai, H. Abe, T. Goto, Y. Yoshimura, S. Kushiyama and H. Matsumoto, J. Phys. Chem. B 112, 9841 (2008). [2] Y. Imai, H. Abe and Y. Yoshimura, J. Phys. Chem. B 113, 2013 (2009).

3:10 PM Invited
Synchrotron High-Energy X-Ray Study of Advanced Materials with Nano-Scale Structures: *Yang Ren*[1]; Valeri Petkov[2]; Yandong Wang[3]; Zhihua Nie[3]; Dongmei Liu[4]; Peter Liaw[5]; [1]Argonne National Laboratory; [2]Central Michigan University; [3]Beijing Institute of Technology; [4]Northeastern University; [5]University of Tennessee

Materials with nano-scale structures have a broad range of applications and detailed knowledge of their atomic-level structure is essential in order to understand and predict their properties and functionalities. Nano-scale structures include nano-particles, nanocrystalline metals and alloys, nano-size precipitates in bulk samples, nano-twins, defects and local disorders, etc. Synchrotron high-energy x-rays are widely used to study the structure, phase transformation and mechanical properties of nano-materials. Among them, a non-traditional approach based on high-energy x-ray total diffraction and atomic pair distribution function data analysis and structure simulations has been developed to investigate the atomic level structures of nanomaterials, that can be performed in various conditions, In this talk, we will present our recent work in this area, including the principle of the method, experimental facility and scientific results of different nanostructures. (Use of the Advanced Photon Source was supported by the U. S. DOE, Office of Science, under Contract No. DE-AC02-06CH11357.)

3:30 PM Invited
Unlocking the 'True' Structure of Complex Materials Using Total Scattering: *Thomas Proffen*[1]; [1]Los Alamos National Laboratory

Total scattering is becoming crucial tool to understanding the atomic structure of complex materials. Conventional structure determination based on Bragg scattering and yields the average structure of the material. However, many modern materials owe their properties to defects or their nano-crystalline character makes conventional Bragg analysis difficult or impossible. New neutron and X-ray instrumentation as well s advances in data reduction and modeling software are making total scattering analysis more accessible and add an invaluable characterization tool for complex materials. Recent developments as well as a cross section of recent applications of this technique will be discussed.

3:50 PM
X-Ray Diffraction Investigation of Ferroelectric Constitutive Behavior at Multiple Length Scales: Goknur Tutuncu[1]; Mesut Varlioglu[1]; Ulrich Lienert[2]; *Ersan Ustundag*[1]; [1]Iowa State University; [2]Argonne National Laboratory

The complex response of ferroelectrics to electromechanical loading requires rigorous characterization of their internal stresses and texture at multiple length scales to fully appreciate their constitutive behavior. *MACROSCALE*: Lattice strain and domain switching (texture) in polycrystalline BaTiO3 under electric field and/or mechanical loading were measured along multiple directions simultaneously. It was seen the lattice strain data are highly anisotropic resulting in large differences between hkl-specific strains. In addition, texture analysis suggests non-180° domain switching is tightly coupled with lattice strain evolution. *MESOSCALE*: The 3D-XRD X-ray diffraction technique was employed to probe the constitutive behavior of individual grains of polycrystalline BaTiO3 under electric field. In addition, domain variants of those grains were identified and their evolution was monitored as a function of applied field and temperature. 3-D XRD data correlate well with the macroscale results, but also yield valuable information about local variations at the mesoscale.

4:05 PM
Imaging Strains on the Nanoscale with Coherent X-Ray Diffraction Microscopy: *Ross Harder*[1]; Loren Beitra[2]; Steven Leake[2]; Marcus Newton[3]; Ian Robinson[2]; [1]Argonne National Lab; [2]University College London; [3]University of Surrey

Nanocrystals are being developed for a great range of applications. Strain on the nanometer scale within these structures has a great impact on their electronic properties. Coherent x-ray diffraction(CXD) microscopy done around the Bragg peaks of nanocrystalline samples have shown remarkable sensitivity to strain within the crystal structure. Recent improvements in CXD instrumentation at the Advanced Photon Source have allowed us to measure CXD patterns around multiple Bragg peaks of isolated nanocrystals of gold and zinc oxide. When each of these Bragg peaks is inverted to direct space the 3D image contains one projection of the distortion of the nanocrystal lattice within the crystal. These separate images have been combined into a fully three-dimensional image of the distortion field of the lattice of the nanocrystals. The full strain tensor of the material in 3D can then be visualized. Our imaging of the strain within nanocrystals will be discussed.

4:20 PM Break

4:30 PM Invited
Geometry, Topology and Structure of Amorphous Solids: *Zbigniew Stachurski*[1]; Richard Welberry[1]; [1]Australian National University

The understanding of the structure of solids began with the concept of translational symmetry, and has to a large degree come about because of the methods of X-ray crystallography. Frank and Kasper considered the topology of clusters of atoms instead of crystallographic unit cell. They distinguished three cases: (1) Coordination shell atoms make equilateral triangles with the centre. (2) Triangles in coordination shell are equilateral; shell atoms make isosceles triangles with the centre. (3) No requirements on the shape of the triangles within the shell. The third case provides a basis for development of a model of a completely random structure (ideal amorphous solid). A model of Zr-based metallic glass has been constructed and described. Debye x-ray scattering computations can reveal the presence of vacancies and other imperfections. Two new atomic mechanisms are identified as the fundamental means of compositional re-distribution in the alloy.

4:50 PM Invited
In-Situ Neutron Diffraction Study of B2 CoTi and CoZr: Rupalee Mulay[1]; James Wollmershauser[1]; *Sean Agnew*[1]; [1]University of Virginia

Fully-ordered B2 intermetallic compounds, CoTi and CoZr, are examined by in-situ neutron diffraction during compression testing. The results reiterate that the primary slip systems in these materials are <100> {011}, but also exposed a deformation mechanism transition that helps to explain the anomalous ductility of these compounds. Previous studies revealed kink banding, under some conditions. Preliminary cyclic tension tests carried out on these materials have shown that they exhibit a strong Bauschinger effect, and recent publications in the literature have emphasized a possible connection between "incipient kink banding" and such strong Bauschinger effects. However, preliminary polycrystal plasticity modeling predicts a similarly strong Bauschinger effect in CoZr without the incorporation of a kink banding mechanism, rather intergranular stresses create the effect. Cyclic in-situ neutron diffraction and electron back-scattered diffraction studies of CoTi and CoZr are being used to determine the role of kink banding in the deformation of these materials.

5:10 PM
Influence of Calcium and Strontium Substitution on the Expansion Behaviors and Oxygen Vacancy Concentration of the Lanthanum Ferrite: *David Thomsen*[1]; Patrick Price[1]; Ellen Rabenberg[1]; Darryl Butt[1]; [1]Boise State University

X-ray diffraction (XRD) was used to investigate the lattice expansion behavior of LaxCa1-xFeO3-d and LaxSr1-xFeO3-d which are mixed ion conductor. LaxCa1-xFeO3-d and LaxSr1-xFeO3-d samples were made by solid state method from 0 = x = 1. The Bruker AXS D8 Discover high-resolution XRD was used to measure the lattice as a function of temperature. XRD has the ability to isolate the lattice parameter with negligible effect from changing vacancy concentration. By comparison, dilatometry measures bulk thermal expansion, which includes the effects of vacancies. In theory, the vacancy concentration in the material can be determined from the difference between the two methods of measurement. Substitution of Ca2+ can influence the thermal expansion both by creating oxygen vacancies and affecting local lattice distortions. Detailed expansion behavior of LaxCa1-xFe3-d and LaxSr1-xFeO3-d as a function of temperature and composition was developed by comparing data from dilatometry and XRD patterns.

5:20 PM
Application of Small Angle Neutron Scattering to Study the Nucleation and Growth Mechanisms of Thin and Thick Films: *Yong Choi*[1]; B. S. Seong[2]; E. J. Shin[2]; [1]Sunmoon University; [2]KAERI

Small angle neutron scattering was applied to non-destructively analyze microstructure of various thin and thick films for electronic and automobile industries and to study the nucleation and growth mechanisms of the electro-deposited films. Average thickness of nano-sized multi-layers of thin film device was non-destructively evaluated by SANS model. Eco-friendly trivalent chromium layers have nano-sized cracks about 40 nm in size, which decreased with decreasing plating current density and voltage. The micro-size crack with "Calabash shape" is formed by the interconnection of the several nano-sized cracks. A nucleation and growth model of the trivalent chromium layers under pulse current condition was proposed based on the microstructure observation and SANS results.

5:35 PM
Non-Destructive Evaluation of Crack Size and Distribution of Eco-Friendly Trivalent Chromium Deposits for Automobile Industries by Small Angle Neutron Scattering: *Yong Choi*[1]; Sik C. Kwon[2]; Eun J. Shin[3]; Baik S. Seong[3]; [1]Sunmoon University; [2]KIMS; [3]KAERI

Eco-friendly trivalent chromium layers was prepared in a modified chromium sulfate bath by various electroplating conditions to replace hexavalent hard chromium coating in industrial fields, which microstructure were analyzed by small angle neutron scattering (SANS) and electron microscopy, respectively. The deposit has columnar grains in which chromium clusters and inter-connected cracks existed. Most of nano-size crack in a grain has about 40 nm in size. The crack size was decreased with decreasing plating current density and voltage. The interconnected micro-size crack seems to be "Calabash shape" which is formed by the interconnection of several nano-size cracks. A nucleation and growth model for the pulse plated chromium layer will be proposed based on the SANS and microstructure observation.

5:50 PM
EXAFS Measurements in Fe-Based Magnetostrictive Single Crystals: *Gavin Garside*[1]; Shamita Shitole[1]; Sivaraman Guruswamy[1]; [1]University of Utah

Magnetostriction is sensitive to the inter-atomic spacing of the magnetic ion core in ferromagnetic materials. Measurements of local inter-atomic distances is of interest to gain an improved understanding of how solutes influence magnetostriction in alpha-Fe-based alloys. Extended x-ray absorption fine structure (EXAFS) measurements were made at the Advanced Photon Source at ANL on Fe-X (where X= Ga, W, and Mo) based single crystals of specific composition and thermal history, that show large magnetostriction. These measurements were made at the K-edges of Fe and the L-edges for W and Mo, to determine the Fe-X, Fe-Fe, and X-X atom distances and short range ordering pair correlations to help understand how Ga, W, and Mo additions modify the magnetostriction of Fe.

Nuclear Energy: Processes and Policies: Characterization

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS/ASM: Nuclear Materials Committee, TMS: Public and Governmental Affairs Committee
Program Organizers: Brajendra Mishra, Colorado School of Mines; Aladar Csontos, U.S. Nuclear Regulatory Commission; Stuart Maloy, Los Alamos National Laboratory; Jeremy Busby, Oak Ridge National Laboratory; Sue Lesica, U.S. Department of Energy's Office of Nuclear Energy

Wednesday PM — Room: 201
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Todd Allen, Idaho National Laboratory; Aladar Csontos, US Nuclear Regulatory Commission

2:00 PM Keynote
Characterization of Neutron- and Ion-Irradiated Nano-Structured Ferritic Alloys by TEM: *James Bentley*[1]; David Hoelzer[1]; [1]Oak Ridge National Laboratory

Nano-structured ferritic alloys (NFA) have outstanding mechanical properties and the potential to be highly resistant to radiation damage through the presence of high concentrations (>10^{23} m^{-3}) of small (<5 nm) Ti-Y-O nanoclusters (NC). Energy-filtered transmission electron microscopy (EFTEM) is essential for reliable characterization of NC by TEM. Our continuing studies involve characterization of neutron-irradiated specimens, including 12YWT and MA957 irradiated in HFIR to 9 dpa at ~500°C, and in-situ ion irradiations of NFA, including 14YWT, to observe directly the effects of irradiation on individual NC. EFTEM characterization of 14YWT before and after ion irradiation at the Argonne National Laboratory IVEM-Tandem Facility will be supplemented by in-situ irradiation with concurrent EFTEM at the French JANNuS facility. Research supported by the Division of Materials Sciences and Engineering and the SHaRE User Facility of the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

2:35 PM
A Multilab-Multitechnique SANS, APT and TEM Characterization Study of a Reference Nanstructured Ferritic Alloy: *G. Robert Odette*[1]; Nicholas Cunningham[1]; Yuan Wu[1]; Erin Haney[1]; Emmanuelle Marquis[1]; Peter Hosemann[1]; Eric Stergar[1]; [1]UC Santa Batrbara

Future energy systems require structural alloys with outstanding properties that are sustained during long-term service in ultra-severe environments. We are developing a new transformational class of nanostructured ferritic alloys (NFA) that show enormous promise for meeting these challenges. NFA are 12-14 Cr steels that are powder processed by dissolving Y and O by ball milling. These elements precipitate along with Ti during hot consolidation to form an ultra-high density of Y-Ti-O-enriched nano-features (NF), that produce very high strength, are remarkably stable, trap He in fine-scale bubbles and enhance vacancy-self interstitial atom recombination, suppressing severe radiation damage. However, the precise characters of various NF are not yet well understood; they appear to range from complex clusters with Y,Ti,O – Ti,O core-shell shells structures to near stoichiometric complex oxides. This presentation will update progress on a round robin characterization study of a reference NFA by SANS, APT and TEM.

3:00 PM
Characterization of 14YWT As Atomized, Milled and Annealed Powders and Consolidated Alloys: *Nicholas Cunningham*[1]; Yuan Wu[1]; G. Robert Odette[1]; Erin Haney[1]; [1]UC Santa Barbara

Fourteen Cr nano-dispersion strengthened ferritic alloys, that contain a high density of Y-Ti-O-enriched nano-features (NF), have high strength, are very stable and manifest remarkable radiation damage tolerance. A multi-technique characterization of 14Cr-0.2T-0.3Ti-low to 0.015O powders obtained from Crucible Research (as part of a collaborative study with LANL, ORNL, UC Berkeley and South Dakota School of Mines and Crucible Research) is described. Powders were characterized in the as-atomized, milled, annealed and consolidated conditions using EMPA, SANS, APT, TEM and microhardness methods. Special emphasis was on characterizing the distribution of Y after various processing steps and the distribution and character of NF after heat treatment and their relation to the alloy grain size distribution and strength. Inhomogeneous Y distributions in the as-atomized powders are homogenized by milling. Powder annealing and hot consolidation result in high concentrations of NF even in cases with bimodal grain size distributions.

3:25 PM

Development and Characterization of Radiation Tolerant Nanostructured Ferritic Steels: *Michael Miller*[1]; David Hoelzer[1]; Kaye Russell[1]; [1]ORNL

The development of advanced materials for future generation power systems requires experimental microstructural characterization of candidate materials to ensure that the microstructure, and hence the properties, remain stable during exposure to high doses of irradiation at elevated temperatures. The atomic level quantification of the microstructural features provided by atom probe tomography enables a fundamental understanding of the nanostructured ferritic steels to be established and provides the necessary scientific background for future regulatory guidelines. The unique stability of 2-4-nm-diameter Ti-O-Y nanoclusters in nanostructured ferritic steels that were exposed to high doses of neutron and ion irradiations will be discussed. This research was sponsored by the Division of Materials Sciences and Engineering and the SHaRE User Facility of the Scientific User Facilities Division in the Office of Basic Energy Sciences, U.S. Department of Energy.

3:50 PM Break

4:05 PM

Characterization of Nano-Scale Particles in Mechanically Alloyed and HIP-ed Oxide Dispersion Strengthened Steels: *Dhriti Bhattacharyya*[1]; Patricia Dickerson[1]; Peter Hosemann[1]; G. Odette[2]; Michael Nastasi[1]; Amit Misra[1]; Stuart Maloy[1]; [1]Los Alamos National Laboratory; [2]University of California, Santa Barbara

Oxide Dispersion Strengthened (ODS) ferritic steels with a high density of nano-features, also known as Nano-structured Ferritic Alloys (NFAs) have excellent potential to withstand high doses of radiation when used in advanced fission and fusion reactors. The nano-features thought to be responsible for the exceptional radiation damage tolerance in these steels are complex oxides of Y and Ti, the detailed structure and chemistry of which are not fully understood. Two such ODS alloys are: a commercially produced mechanically alloyed steel MA-957 (produced by Special Metals), and a recently developed alloy, U14YWT, which, for this heat, is processed by Hot Isostatic Pressing (HIP). In this work, the authors examine the morphology, crystal structure and chemistry of various kinds of nano-scale oxide particles existing in these alloys and their orientation relationship with the BCC iron matrix using conventional and high-resolution Transmission Electron Microscopy (TEM) and Energy Dispersive X-Ray Spectroscopy (EDX).

4:30 PM

TEM Characterization of a Monolithic U-Mo Plate-Type Nuclear Fuel: *Dennis Keiser*[1]; JanFong Jue[1]; Bo Yao[2]; Emmanuel Perez[2]; Yongho Sohn[2]; [1]Idaho National Laboratory; [2]University of Central Florida

The Reduced Enrichment for Research and Test Reactors (RERTR) program is developing low-enriched U-Mo alloy fuels for application in research and test reactors. One type of fuel is a monolithic plate-type fuel where a U-Mo foil is co-rolled with Zr and then encased in 6061 Al cladding. The starting microstructure of the fuel plate after fabrication will impact the performance of the plate in reactor. As a result, a TEM investigation has been performed on as-fabricated fuel plates to determine the phases that developed at the U-Mo/Zr and Zr/6061 Al cladding interfaces during the hot isostatic pressing (HIP) fabrication process. This talk will describe the types of phases that were identified and how these phases can impact the performance of the fuel plate during irradiation. Some actual images of irradiated fuel plates will be presented to demonstrate how different phases behaved during irradiation.

4:55 PM

Weldability Characteristics of Oxide Dispersion Strengthened Alloys: An Overview: *Kalyan Chitrada*[1]; Ramprashad Prabhakaran[2]; Jiye Wang[3]; Larry Zirker[2]; Mitchell Meyer[2]; James Cole[2]; Korukonda Murty[4]; Rajiv Mishra[3]; Darryl Butt[5]; Megan Frary[5]; Indrajit Charit[1]; [1]University of Idaho; [2]Idaho National Laboratory; [3]Missouri University of Science and Technology; [4]North Carolina State University; [5]Boise State University

Oxide dispersion strengthened (ODS) alloys are considered an important class of structural materials for various high temperature applications including advanced nuclear reactors. Conventional fusion welding methods lead to high porosity and agglomerated oxide particles in these alloys deteriorating critical properties of the joint. That is why solid state joining techniques are touted as the potential remedy for the welding issues encountered in these alloys. Research activities in an ongoing research program supported by the DOE (grant # DE-FG07-08ID14925) are highlighted. In this program, friction stir welding and pressure resistance welding have been used to successfully weld various ODS alloys, such as MA956, MA957 and MA754. Microstructural characteristics of the welded alloys are studied using a host of microscopy techniques. Mechanical properties are evaluated using microhardness, miniaturized tensile and shear punch test techniques. Appropriate microstructure-property correlations are developed. An overview of the state-of-the-art based on the published literature is also presented.

5:20 PM

Multi-Scale Characterizations and Formation Mechanism in an ODS Steel Elaborated by Reactive Ball-Milling and Annealing: *Mathilde Brocq*[1]; Fabrice Legendre[1]; Bertrand Radiguet[2]; Marie-Hélène Mathon[3]; Fabien Cuvilly[2]; Philippe Pareige[2]; [1]SRMP - CEA; [2]GPM-Université de Rouen; [3]LLB

Oxide dispersion strengthened (ODS) steels are promising structural materials for future nuclear reactors. Indeed they exhibit excellent creep and radiation resistance thanks to a dispersion of complex nanometric oxides. We proposed a new processing route based on reactive ball milling of iron oxide (Fe_2O_3), yttria intermetallic (YFe_3) and iron based alloy. A multiscale characterization including Atom Probe Tomography (APT) and Small Angle Neutron Scattering (SANS) was performed.In as-milled material, Y, Ti and O enriched nanoclusters were observed. From 400°C up to 800°C annealing, the nanocluster density increases while their size remains unchanged. In those synthesis conditions, a new formation mechanism is highlighted. Indeed not only nanocluster nucleation starts during ball-milling but also their number greatly increases thanks to brief and low-temperature annealings. This is not a usual dissolution-precipitation mechanism lead by thermodynamic. As a conclusion another mechanism based on ball-milling property of creating metastable state will be proposed.

Pb-Free Solders and Emerging Interconnect and Packaging Technologies: Microstructure, Intermetallics, Whisker(I)

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Electronic Packaging and Interconnection Materials Committee

Program Organizers: Kwang-Lung Lin, National Cheng Kung University; Sung Kang, IBM; Jenq-Gong Duh, National Tsing-Hua University; Laura Turbini, Research In Motion; Iver Anderson, Iowa State University; Fu Guo, Beijing University of Technology; Thomas Bieler, Michigan State University; Andre Lee, Michigan State University; Rajen Sidhu, Intel Corporation

Wednesday PM — Room: 204
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: John W. Morris, University of California-Berkeley; Andre Lee, Michigan State University

2:00 PM

A Quantitative Assessment of Microstructural Coarsening of SnAgCu Solders: Effect of Metallization and Thermo-Mechanical History: *Praveen Kumar*[1]; Zhe Huang[1]; Indranath Dutta[1]; Ganesh Subbarayan[2]; Vikas Gupta[3]; [1]WSU; [2]Purdue University; [3]Texas Instruments

Microstructural coarsening in small Sn-3.8%Ag-0.7%Cu joints attached to Ni bond-pads and bulk solder samples, subjected to various thermo-mechanical histories, was quantitatively characterized. The Ag_3Sn precipitates coarsened significantly faster in smaller joints as compared to the bulk samples, and the coarsening was more rapid nearer the bond-pads than farther away. This accelerated aging was attributed to the depletion of Cu from the joint samples due to solution/reaction with Ni pads. In addition to precipitate coarsening, the volume fraction of the eutectic-microconstituent also increased due to aging, leading to an accelerated increase in the inter-particle spacing. Based on these observations, we define a thermo-mechanical history dependent effective diffusion distance, on which precipitate spacing within the eutectic depends linearly. This proffers a single length parameter which may be used to describe in situ evolution of constitutive behavior due to precipitate coarsening during any thermo-mechanical history.

2:15 PM
Interfacial Reactions of Sn3.0Ag0.5Cu Solder with Cu-Mn UBM during Aging: *Chien-Fu Tseng*[1]; Jeng Gong Duh[1]; [1]National Tsing Hua University

Cu UBM has been widely used as surface finish in the filp chip technology. The major disadvantages of Cu UBM are fast consumption of copper, rapid growth of IMCs and formation of Kirkendall voids. Recently, minor element addition into Cu UBM has been observed to suppress the formation of Cu-Sn IMCs at the interface. In this study, different Mn content (1-20 at.%) were added into Cu UBM by sputtering technique. With higher Mn concentration in Cu-Mn UBM, a new phase, MnSn2, was formed between Cu6Sn5 and Cu-Mn UBM. MnSn2 may be a diffusion barrier to reduce the interfacial reaction and reduce the formation of kirkendall voids. The detailed mechanism of the IMC formation will be probed and discussed.

2:30 PM
Cross-Interaction between Ni and Cu across a High-Lead Solder Joint with Different Solder Volume: *Chih-Chiang Chang*[1]; C. Robert Kao[1]; [1]National Taiwan University

In this study, the Ni/95Pb5Sn/Cu ternary diffusion couples were used to investigate the solder volume effect on the cross-interaction between Ni and Cu. Experimentally, a high-lead solder layer with thickness of 100 or 400 microns was electroplated over Cu foils. A pure Ni layer (20 microns) was then deposited over the as-deposited high-lead solder surface. The diffusion couples were aged at 150 to 250°C for different periods of time. With this technique, the diffusion couples were assembled without experiencing any high temperature process, such as reflow, which would have accelerated the interaction and caused difficulties in analysis. This study revealed that the massive spalling also occurred in aging state without reflow. The massive spalling stared from the formation of the micro-voids. When the micro-void congregated, the intermetallics (Cu3Sn) stared to spall from the interface. This spalling phenomenon will occurred early due to higher aging temperature and smaller solder volume.

2:45 PM
Current Stressing Effect on Intermetallic Compound Growth Kinetics in Cu Pillar/Sn Bump: Myeong-Hyeok Jeong[1]; Jae-Won Kim[1]; Gi-Tae Lim[1]; Byoung-Joon Kim[2]; Kiwook Lee[3]; Jaedong Kim[3]; Young-Chang Joo[2]; *Young-Bae Park*[1]; [1]Andong National University; [2]Seoul National University; [3]Amkor Technology Korea Inc

Cu pillar bump makes large amount of intermetallic compound and Kirkendall void between Cu pillar and solder which can degrade electrical and mechanical reliability. Therefore, it is essential to understand the fundamental growth mechanisms of intermetallic compound and Kirkendall void. In this work, we performed kinetic studies on the Cu pillar/Sn bump structure in order to quantify the amount of intermetallic compound and Kirkendall void by using in-situ annealing and electromigration test in a scanning electron microscope chamber during current stressing conditions with current density of 3.5~7.2x104 A/cm2 at 120~180°. The activation energy values for the growth of Cu6Sn5, Cu3Sn, and total (Cu6Sn5+Cu3Sn) IMC were found to be 0.16, 0.56 and 0.48 eV/atom, respectively. Current density exponent for transition time of IMC during current stressing was estimated to be 2.2. And also, their effects on the electrical reliability of Cu pillar bump during current stressing will be discussed in detail.

3:00 PM
Formation and Growth of Intermetallic Compound (Cu_6Sn_5) at Early Stages in Lead-Free Soldering: *Min Soo Park*[1]; Raymundo Arroyave[1]; [1]Texas A&M University

Phase field simulations of Intermetallic compound (IMC) formation and growth during early stages will be performed, considering the interactions between liquid Sn-based solder and copper substrate. The liquid Sn-based solder (L phase) and the copper substrate (α phase) are considered to be under metastable conditions that eventually lead to the nucleation of Cu_6Sn_5 IMC (η phase) at the interface between the two substances. The nucleation events are determined by using a classical nucleation theory represented probabilistically through Poisson distribution function. The driving force can be calculated from the Gibb's energies through the CALPHAD approach. Phase field simulations for nucleation phenomenon at the early stages will be prepared with variation of phases' according to temperatures and L/η interface energies to numerically investigate the possible soldering reactions at the early stages compared with previous works, showing the decomposition of the substrate and the formation and growth (or coalescence) of IMC grains.

3:15 PM
Local Mechanical Properties of Cu6Sn5 Intermetallics in Pb-Free Solder Joints by Microcompression Testing of Pillars: *Ling Jiang*[1]; Nik Chawla[1]; [1]Arizona State University, School of Mechanical, Aerospace, Chemical, and Materials Engineering

A methodology for performing uniaxial compression tests on Cu6Sn5 intermetallics in Pb-free solder joints was used to probe mechanical properties of Cu6Sn5 intermetallics. Focused Ion beam (FIB) was employed to mill Cu6Sn5 pillars in various nodules grown between Sn-rich solder and a Cu substrate. The pillars were tested using a nanoindenter with a flat tip in compression, to determine the stress-strain behavior of the Cu6Sn5 pillars. Young's modulus of Cu6Sn5 intermetallics obtained in uniaxial compression testing was compared with that obtained by nanoindentation. The effect of aspect ratio and taper of pillars on mechanical properties will be discussed. The crystallographic orientation of pillars was examined using electron back-scattered diffraction. The relationship between orientation and mechanical properties of pillars will be discussed.

3:30 PM Break

3:45 PM
Effects of Minor Ni Doping on Interfacial Reaction and Microstructure Variation in the Cu/Sn-3Ag-0.5Cu-xNi/Au/Ni Sandwich Structure: *Chi-Yang Yu*[1]; Jenq-Gong Duh[1]; Tae-Kyu Lee[2]; Michael Tsai[2]; Kuo-Chuan Liu[2]; [1]National Tsing Hua University; [2]CISCO

Cu/Sn-3Ag-0.5Cu-xNi/Au/Ni (x= 0, 0.01, 0.05 and 0.1 wt.%) after reflow were aged at 100 oC and 150 oC, respectively, for 500 h. In the consideration of interfacial reaction, the local Ni concentration would affect the formation of intermetallic compounds (IMCs), i.e. (Cu,Ni)6Sn5 and (Ni,Cu)3Sn4. The behavior of Ni migration before and after aging at different temperature was investigated with the aid of field emission electron probe microanalyzer (FE-EPMA). It was revealed that the morphology and growth rate of IMCs at both Cu and Au/Ni sides were rather different. During the heat treatment, cross-interaction was attributed to the Cu and Ni diffusion from one side to the other side between Cu and Au/Ni substrates. The variation in elemental distribution would cause microstructure evolution in these solder matrixes. In this study, the effects of minor Ni doping on interfacial reaction and microstructure variation in the solid state reaction will be reported.

4:00 PM
Mechanical Properties of Interfacial IMCs in Solder Joints Evaluated by Nanoindentation: *Y.L. Shen*[1]; C. W Su[2]; J. M. Song[2]; S. Y. Chen[1]; [1]National Taiwan University of Science and Technology; [2]National Dong Hwa University

This study reports the mechanical properties of the intermetallic compounds (IMCs) formed at the interfaces between Sn-Ag-Cu, Sn-Zn solders and the commonly used electronic substrates using nanoindentation. The hardness (H), elastic modulus (E), yield strength (Y) and work hardening exponent (n) were estimated. In view of the reliability under the conditions of drop or creep, strain rate sensitivity (m) and creep stress exponent (CSE) of the interfacial IMCs were also evaluated. Results showed that soft Ag and Au based IMCs exhibited a greater degree of strain rate hardening compared to hard Cu and Ni based IMCs. With respect to creep properties, it could be concluded that the CSE value was in agreement with the work hardening exponent (n) rather than melting temperature or crystal structure. This implies that IMCs with greater dislocation slip resistance exhibited better ability against creep.

4:15 PM
Kinetics of Intermetallic Compound Formation at the Interface between Sn-3.0Ag-0.5Cu Solder and Cu-Zn Alloy Substrate: *Youngmin Kim*[1]; Hee-Ra Roh[1]; Young-Ho Kim[1]; [1]Hanyang University

The interfacial reaction and intermetallic compound (IMC) growth during aging at the Sn-3.5Ag-0.5Cu (SAC)/Cu-Zn interface were investigated. By dipping Cu or Cu-10Zn wires into the molten solder at 260°, the scallop-shaped Cu_6Sn_5 formed. Then, specimens were aged subsequently at 120°, 150°, and 180° up to 2000 h. The typical bi-layer of Cu_6Sn_5 and Cu_3Sn formed and numerous microvoids were found at the SAC/Cu interfaces, while no Cu_3Sn and microvoids were observed at the SAC/Cu-Zn interfaces after aging. IMC growth was remarkably depressed on Cu-Zn substrates and this effect was more prominent at higher aging temperature. The parabolic behavior of IMC thickness versus aging time shows the IMC growth is controlled by diffusion. The activation energy for the IMC growth of SAC/Cu-Zn specimens was larger than that of SAC/Cu specimens. This research was supported by the Component Material Technology Development Program of the Ministry of Commerce, Industry, and Energy (MOCIE).

4:30 PM
Sn Whiskers and Grain Boundary Sliding: *John Osenbach*[1]; [1]LSI Corporation

Grain boundary sliding has been proposed as one possible mechanism for whisker nucleation and growth. Experimental results are presented indicating grain boundary sliding prevents whisker growth rather than promoting whisker growth. It will be shown that these results are consistent with the predictions of a multi-mechanism creep/whisker theory.

4:45 PM
Critical Current Density of Inhibiting the $(Cu,Ni)_6Sn_5$ Formation in the Ni-Side of Cu/Solder/Ni Joints: W.H. Wu[1]; H.L. Chung[1]; C.N. Chen[1]; *Cheng-En Ho*[1]; [1]Yuan Ze University

The Cu/solder/Ni sandwich structure is one of the most common joint configurations used to electrically connect chips to the next packaging level. During joints operation, the Cu can diffuse across the entire solder region and nucleates as an undesired $(Cu,Ni)_6Sn_5$ layer over the Ni-side of Cu/solder/Ni. The driving force for this cross-interaction process is known to be the chemical potential gradient. To counterbalance the chemical force-induced Cu flux, an opposite current stressing with various current densities (0 - 2 \215 10^4 A/cm^2) was examined using a Cu/Sn(50 microns thick)/Ni structure at a fixed specimen temperature, 150 Celsius. Research results clearly indicated the growth of $(Cu,Ni)_6Sn_5$ cannot be retarded until a current stressing of near 10^4 A/cm^2 is applied. This suggests that the critical current density of inhibiting the $(Cu,Ni)_6Sn_5$ formation is approximately 10^4 A/cm^2. The strong correlation between the $(Cu,Ni)_6Sn_5$ growth and current densities will be presented in this study.

5:00 PM
Interfacial Reactions between near Eutectic Snagcu Solder Alloys and Electrolytic Au/Ni Substrates: *Mao Gao*[1]; Eric Cotts[1]; [1]Binghamton University

Interfacial reactions during reflow between near eutectic SnAgCu solder and Au/Ni substrates profoundly affect final solder joint microstructure. Reaction products and morphologies are affected not only by time and temperature of anneals, but by small changes in the concentration of the noble metals in the solder. Such dependencies were examined for a range of conditions using differential scanning calorimetry to impose a precise thermal history upon the samples. Quantitative relationships between the growth kinetics of both (Cu,Ni,Au)6Sn5 and (Ni,Cu)3Sn4, and the initial Cu supply (Cu concentration and solder volume), and the thermal conditions were examined. As previously observed, for high Cu concentrations, (Cu,Ni,Au)6Sn5 initially formed at the SnAgCu/Ni interface. When the Cu concentration in the solder decreased to 0.32% wt., (Ni,Cu)3Sn4 was observed to form at the (Cu,Ni,Au)6Sn5 /Ni interface. Under certain conditions, the (Cu,Ni,Au)6Sn5 intermatellic layer or (Ni,Cu)3Sn4 was observed to spall at the interface.

5:15 PM
Effect of Ag on the Kirkendall Void Formation in Sn-Ag/Cu Solder Joints: *Sunghwan Kim*[1]; Jin Yu[1]; [1]KAIST

Sn-Ag solders with varying amount of Ag were reacted with Cu UBM which was electroplated using an additive containing S. After the reflow process, all specimens were isothermally aged at 150 C for varying times. Developments of Kirkendall voids at the joints were investigated using SEM, while variation of the surface chemistry of the joint interfaces were monitored using AES. It was shown that reduction of the Ag content below the eutectic composition allowed more S segregation at the Cu3Sn/Cu interface, which is concomitant with larger fraction of Kirkendall voids at the interface. This is consistent with our recent analyses on the effect of sulphide forming element additions to Sn-3.5Ag solder on the Kirkendall void formation (Acta Mater. in press).

Polymer Nanocomposites: Metals and Other Nanoparticles

Sponsored by: The Minerals, Metals and Materials Society
Program Organizer: John Zhanhu Guo, Lamar University

Wednesday PM — Room: 309
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Katie Weihong Zhong, Washington State University; Qiang Wang, Institute of Chemical and Engineering Sciences (ICES); Lu Sun, Praxair Electronics

2:00 PM Introductory Comments

2:05 PM Keynote
Effect of Particle Size on the Strength of Nanocomposites: *C. T. Sun*[1]; [1]Purdue University

The particle size effect on the mechanical properties of nanocomposites has not been convincingly established because the quality of particle dispersion in nanocomposites cannot be assured. Thus, it is difficult to decouple the effect of nanoparticle size and its dispersion on the mechanical properties of nanocomposites made from conventional processing methods. Moreover, particle dispersion is also affected adversely as the loading (weight/volume fraction) of nanoparticles increases. In this talk, the effect of particle size on the mechanical properties of polymeric nanocomposites is examined based on experimental results using a processing method to achieve uniform particle dispersion in an epoxy resin. MD simulation and fracture mechanics are used to aid the interpretation of the experimental results. The fracture toughness of the interfacial crack is evaluated experimentally using micron-sized particles and the size effect is then extrapolated to nanoparticles. The results indicate that debonding is unlikely a failure mode in nanocomposites.

2:45 PM
Electrically Conductive Nanocomposites with Thermoplastic Polymers: *Nathan Hansen*[1]; George Hansen[1]; Greg Sawyer[2]; [1]Conductive Composites Company; [2]University of Florida

Nickel Nanostrands are three dimensional nanostructures with a branching and interconnected geometry, forming a network of metallic nanoscale Faraday cages and three dimensionally percolated networks. As such, the electromagnetic shielding and electrical conductivity properties of polymer nanocomposites using these materials have outstanding properties. Nanostrands are easily dispersed in low viscosity mediums, such as paints and water. However, there have been challenges in dispersing these nanomaterials in highly viscous thermoplastic polymer systems. A novel method of dispersion using jet milled polymer powders allows micron diameter powders to be blended with nanostrand structures. These polymer powders can be dry mixed with nanostrands, or solvated and solution mixed. The resulting conductive powder blend can be used in any commercial thermoplastic polymer process, with composite bulk resistivities of 0.01-0.001 ohm-cm at 10 volume percent filler. Electrical, electromagnetic, percolative, and microanalytical results are presented.

3:05 PM
Effects of Incorporation of Silica and Zirconia Nanoparticles on the Thermal and Thermomechanical Properties of Polymer Nanocomposites: *Muhammad Sajjad*[1]; Thomas Koch[1]; Sabine Seidler[1]; [1]TU Wien

Hybrid materials of PMMA, Polystyrene & Epoxy consisting of Silica and Zirconia nanoparticles with loadings up to 10 % have been characterized by DSC, TGA, DMA and Nanoindentation techniques. Nanocomposites were prepared via in situ polymerization whereas the dispersibility of the particles in organic media was investigated by DLS,SAXS experiments and TEM.We were able to synthesize polymer systems filled with small particles (22 nm in size), aggregated at nanometer size only, and well dispersed large particles (66 nm in size).The properties of the resulting nanocomposites were generally superior to the pure polymer matrix. Composites with strong interface exhibit profound effect on the ultimate properties as clear from the results of high values of damping, glass transition temperature Tg and hardness modulus. The enhanced Tg values observed in the nanocomposites arise from these attractive polymer-nanoparticles interfacial interactions that reduce cooperative segmental mobility. Composites with weak interface showed essentially no change in Tg and damping or even a decline with filler contents. This reduction is ascribed to the free surfaces at the non wetted interfaces of the matrix and nanoparticles that were not well dispersed. The prepared nanocomposite films exhibited somewhat high hardness, better transparency and good thermal stability. On the other hand, incorporation of the particles did not alter the thermal degradation behaviour of PMMA and Epoxy.

3:25 PM
Electrical Resistance Investigation of Cotton Fabrics after Treating with Polyaniline Solution: *Cem Gunesoglu*[1]; Sinem Gunesoglu[1]; Suying Wei[2]; Zhanhu Guo[2]; [1]Gaziantep University; [2]Lamar University

The emanating electromagnetic radiation has become serious concerns, not only for increased working quality of devices but also for health. Any protection by textiles needs certain electrical conductivity; however, traditional fibers used in the textile fabrics are electrically insulating materials with a negligible electromagnetic shielding performance. The widely accepted technique is to add conductive fillers into the textile fabrics to manufacture conductive woven or knitted fabrics. However, macrostructure will have large effect on constructional properties like thickness, weight and appearance. Highly conductive textile surface will need micron and nano conductive fillers considering the minimal changes of the fabric properties. This study investigates the usage conductive polymeric nanocomposites such as polypyrrole (PPy) and polyaniline (PANI) to increase the electrical conductivity of textile fabrics. The production and application of the nanocomposites are discussed, conductivity of treated fabrics is obtained by standard four-probe method and physicochemical property changes of the textile are evaluated.

3:45 PM Break

4:15 PM Invited
Multifunctional Conductive Nanocomposites: Fabrication, Property Analysis and Applications: *John Zhanhu Guo*[1]; Di Zhang[1]; Pallavi Mavinakuli[1]; Jiahua Zhu[1]; Suying Wei[1]; [1]Lamar University

Both carbon-based and conductive polymer-based conductive nanocomposites will be presented in the talk. The electric conductivity of these two systems is investigated from low temperature to room temperature. The electron transport phenomena will be presented. The magnetic properties of the magnetic nanocomposites are investigated and will be presented. The application for sensors is also presented in the talk.

4:40 PM Invited
Magnetic Properties of Some Polyaniline-Based Magnetic Nano-Composites for EMI Applications: *Jayanta Banerjee*[1]; O Perales-Pérez[1]; J. Banerjee[1]; [1]University of Puerto Rico at Mayaguez

Polyaniline(PANI)-based magnetic nano-composites, with Mn-Zn ferrite nano-particles as disperse phase, can be used for EMI shielding applications in electronic devices. In the present paper such PANI composites, having different PANI-Ferrite w/w ratios were prepared under suitable laboratory controlled conditions in order to avoid excessive dissolution of the ferrite and in favor of its dispersion in the polymeric matrix. A particular stoichiometry was chosen because of its highest magnetization value (55emu/g) and susceptibility of 3.645. Using Scherrer's formula the ferrite's average crystallite size was calculated as 10.6 nm. HRTEM, XRD and SQUID analyses confirmed the formation of magnetic nano-composites. The saturation magnetization in the nano-composites varied according to the PANI-Ferrite w/w ratio, without affecting the magnetic susceptibility of the ferrite.

5:05 PM
Effect of Nanometer-Sized Titanium Dioxide on the Piezodielectric Effect of Carbon Fiber Sulphoaluminate Cement Composites: *Cheng Xin*[1]; Wang Shoude[1]; [1]University of Jinan

Carbon fiber sulphoaluminate cement composites prepared by pressing. Its piezodielectric effects with or without nanometer-sized titanium dioxide under uniaxial and cyclic loads were investigated in this paper. The experiment results indicated that nanometer-sized titanium dioxide could improve the sensitivity and repeatability of the piezodielectric effect of carbon fiber sulphoaluminate cement composites. This was related to that nanometer-sized titanium dioxide improved the quantity of the polarization dipole in the carbon fiber sulphoaluminate cement composites.

5:25 PM
Design, Synthesis, and Characterization of Polymer Matrix Nanophosphor Composite Scintillators: *Meredith Barta*[1]; Jason Nadler[1]; Zhitao Kang[1]; [1]Georgia Institute of Technology

Polymer matrix nanophosphor composite scintillators are designed, fabricated and characterized for use in a gamma ray detection materials system. Polymer-matrix composite scintillators can be manufactured far more rapidly and easily in a much wider range of geometric configurations compared to conventional single crystals. The durability of these material systems also provides considerable advantages with respect to impact and environmental sensitivity. Recent results indicate that these scintillators can be fabricated using periodic arrays of high phosphor loading regions surrounded by light pipes. Additional results demonstrate the benefits of refractive index matching and near-UV transparency of the polymer matrix.

5:45 PM
Nano-Moldable Polymer-Ceramic Composite: *Isaac Finger*[1]; [1]University of Florida

Recent advancements in the creation of Group 5b aqueous sol-gels has brought about the discovery of a novel particle generation system incorporating Titanium and Silicon oxides. It has been found that the precipitation of this aqueous particle system with the introduction of a ketonated solvent results in the formation of a ceramic-organic hybrid material. After filtration this material has a temporary plasticity that makes it amenable to molding. We have shown that the molding of this material allows for the reliable reproduction of surface features on the scale of microns. It is shown that the micro-morphologies introduced in the molding process are maintained, with high fidelity, through the calcining and sintering process. Hypotheses on the reactivity and microstructure of the material are presented and possible applications of this material are considered.

6:05 PM Concluding Comments

Processing Materials for Properties: Processing-Microstructure-Properties

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division
Program Organizers: Brajendra Mishra, Colorado School of Mines; Akio Fuwa, Waseda University; Paritud Bhandhubanyong, National Metal and Materials Technology Center

Wednesday PM — Room: 617
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Ramana Reddy, The University of Alabama; John Moore, Colorado School of Mines

2:00 PM Keynote
Materials Processing Augmentation in Hostile Environments for Hydrocarbon Recovery: *Rashmi Bhavsar*[1]; Indranil Roy[1]; Christian Wilkinson[1]; [1]Schlumberger

The rising demand for energy combined with our depleting natural oil and gas reserves has led to oilfield operations being conducted in environments which were formerly considered too harsh. Consequently, there has been a constant demand for improved materials and processes to allow operation in these hostile conditions. Low alloys steels have limited corrosion resistance in CO2 environments and Stainless steels have limited resistance in chlorides, hence nickel based alloys are recommended. Embrittlement, the loss of ductility of a metal due to absorption of H2S or hydrogen, resulting in catastrophic failures, has posed a significant challenge to those designing microstructures capable of surviving such environments. In this presentation, technological advancements in materials from new superalloys, coatings and grain-refined nanocrystalline materials to survive extremes of temperature, pressure and corrosive fluids in the oil and gas industry are highlighted. Surface modifications to refine surface morphology to increase corrosion resistance are also discussed.

2:30 PM
Computational and Experimental Investigation into the Oxidation Behavior of HVOF-Sprayed Cryomilled NiCrAlY Bond Coats: *Kaka Ma*[1]; Jianrong Song[2]; Lianmeng Zhang[2]; Julie Schoenung[1]; [1]University of California, Davis; [2]Wuhan University of Technology

Thermal barrier coating systems (TBCs) have been commonly applied to protect turbine blades against high-temperature corrosion and oxidation. The morphology and the composition of the thermally grown oxide (TGO) layer are known to be crucial to the performance of TBCs. Our previous work has demonstrated that cryomilled NiCrAlY coatings exhibit better oxidation behavior than conventional equivalents. After oxidation, the formation of a uniform alumina layer without the presence of other mixed oxide phases was observed on the surface of the cryomilled coating while the conventional coating exhibited a discontinuous alumina layer as well as mixed oxides consisting of NiO and Ni(Cr,Al)2O4 spinels. In this paper, further investigation into the TGO growth in the HVOF-sprayed conventional/cryomilled NiCrAlY coatings is presented, with a focus on microstructural characterization of both the bond coat and TGO after select heat treament conditions. The oxidation mechanism is discussed from the thermodynamic perspective using Thermo-calc® modeling.

2:50 PM
High Thermal Gradient Directional Solidification and Its Application in the Processing of Nickel-Based Superalloys: *Lin Liu*[1]; [1]Northwestern Polytechnical University

During directional solidification, thermal gradients in front of the liquid-solid interface (G) are important in defining the subsequent cooling rate and the solidification microstructure. An elevated G is frequently demanded, especially in the production of single-crystal superalloys and most metallic materials. In this study, the heat transfer during directional solidification by Bridgman-type directional solidification has been analyzed and a relationship has been established that reflects the effect of alloy properties, process parameters and equipment characteristics on thermal gradients. Based on this relationship, some methods for obtaining high thermal gradients have been developed. By using zone-intensified overheating and liquid-metal cooling, high thermal gradients of up to 800 K/cm were achieved. Application of these methods in the processing of single crystal superalloys indicated that high thermal gradient directional solidification produced more uniform microstructures, less microsegregation and optimized mechanical properties.

3:10 PM Keynote
In Search of Rapid Processing Routes for CIGS Photovoltaic Absorber Materials: *Carelyn Campbell*[1]; [1]National Institute of Standards and Technology

Rapid processing of the α-Cu(In,Ga)Se_2 (CIGS) photovoltaic absorber material is critical for making these solar materials cost-effective. The current processing times must be reduced to less than 2 minutes, while maintaining optimum material properties. Exploration of novel processing routes within this complex system requires combining CALPHAD-based thermodynamic and diffusion mobilities descriptions. Using these multicomponent descriptions enables prediction of reaction pathways for prospective processing sequences. Preliminary thermodynamic and diffusion mobility descriptions for the Cu-In-Ga-Se system will be presented. The diffusion mobility descriptions are derived from both measured unary, binary and ternary tracer, intrinsic and chemical diffusion data and experimentally derived activation energies. The diffusion mobility descriptions are then used to simulate a wide range of model reactions. These simulations provide some insights into potential processing routes with significantly lower processing times.

3:30 PM
Microstructure and Properties of New Wear Resistant Steel with High Strength and High Toughness: *Li Hongbin*[1]; [1]Baosteel

A multi-element wear-resistant low-alloy steel with high strength and high toughness was developed. Microstructure, hardness, tensile properties and impact properties were carried out in order to establish a correlation amongst the parameters and to optimize the microstructural features and mechanical properties for superior wear performance. The results show that the optimal microstructure and mechanical properties were got when quenching at 880~910° and tempering at 160~260°. Fine martensite can be obtained, and the hardness is above 500HB, the tensile strength is above 1700MPa, the yield strength is above 1350MPa, the elongation is above 12%, and the impact energy is about 50J. The results obtained have been supplemented through the characteristics of the worn surfaces, subsurface regions, debris and fractured surfaces. These analyses also helped to understand the operative mechanisms of material removal and failure.

3:50 PM
Enhanced Electrical and Mechanical Properties of the Heat-Treated Cu-Ni-(Si, Ti) Alloys: *Kwangjun Euh*[1]; Seung Zeon Han[1]; Sangshik Kim[2]; Sung Hwan Lim[3]; [1]Korea Institute of Materials Science; [2]Gyeongsang National University; [3]Kangwon National University

Cu-Ni-Si alloys are extensively used as leadframe and connector materials in the electronic devices due to their high strength. However, the electrical conductivity of Cu-Ni-Si alloy is relatively lower than those of other leadframe alloys such as Cu-Fe-P alloys. In order to increase electrical conductivity of Cu-Ni-Si alloy without deterioration of strength, thermomechanical treatment such as rolling and heat treatment can be one of promising candidate process methods. In this study, small amount of Ti was added to promote precipitation of Ni-Si compounds and heat-treated at the various temperature and time. Electrical and mechanical properties simultaneously increased at the early stage of aging. The microstructures and properties of the aged specimens were comparatively analyzed in order to understand the effect of aging process on the property enhancement of the Cu-Ni-(Si, Ti) Alloys.

4:10 PM
Preparation and Mechanical Properties of Nanostructured Cryomilled NiCrAlY Alloy Fabricated by Spark Plasma Sintering: *Jianrong Song*[1]; Kaka Ma[2]; Lianmeng Zhang[3]; Julie Schoenung[2]; [1]University of California - Davis and Wuhan University of Technology, China; [2]University of California - Davis; [3]Wuhan University of Technology, China

NiCrAlY coatings are widely used on turbine blades and vanes for protection against high temperature oxidation and corrosion. Nanostructured cryomilled NiCrAlY powder was consolidated by spark plasma sintering (SPS) to provide bulk samples for in-depth characterization without the microstructural complexities that are generated in thermal sprayed coatings. Heat treatment at select times and temperatures was also carried out. Through microhardness testing, Scanning Electron Microscopy (SEM) and Energy-Dispersive X-ray analysis (EDX), the mechanical properties, microstructure and phase composition of the samples were investigated. The results indicated that there was a strengthening effect in the cryomilled alloy, compared to conventional alloy, because of refinement in the microstructure and the presence of nanostructural features. After heat treatment, the microhardness of the samples decreased, due to changes in the microstructure and phase transformation.

4:30 PM
Thermal History and Mechanical Behavior of PH13-8Mo Fabricated via LENS®: *Jonathan Nguyen*[1]; Baolong Zheng[1]; Yuhong Xiong[1]; William Hofmeister[2]; John Smugeresky[3]; Yizhang Zhou[1]; Enrique Lavernia[1]; [1]University of California, Davis; [2]University of Tennessee Space Institute; [3]Sandia National Laboratories

Laser Engineered Net-shaping (LENS®) is a layer additive manufacturing process of near net shape metallic components from computer aided design (CAD) files. Consequently, numerous reheat cycles of previously deposited material are involved which contribute to the microstructural evolution and significantly affect mechanical behavior of LENS® deposited components. Thermocouples and high speed infrared thermal imaging were used to provide insight into the influence of the overall thermal history and molten pool temperature on the resulting microstructure. SEM, TEM, and OM were used to study microstructural changes under various processing conditions. Tensile and microhardness tests were carried out to evaluate the mechanical behavior of LENS® deposited PH13-8Mo. Overall thermal history and molten pool temperatures and their effects on microstructural evolution and resulting mechanical behavior were investigated to better understand the relationships among process parameters, microstructure, and mechanical behavior of LENS® deposited PH13-8Mo components.

4:50 PM
Transformation Induced Plasticity in Fe-Cr-V-C: *Uta Kuehn*[1]; Jan Romberg[1]; Norbert Mattern[1]; Juergen Eckert[1]; [1]IFW

On the basis of the Fe84.3C4.6Cr4.3Mo4.6V2.2 high speed tool steel, manufactured under relatively high cooling rates and highly pure conditions, a further improvement of the mechanical characteristics by slight modification of the alloy composition was attempted. For this, the alloy Fe88.9Cr4.3V2.2C4.6 was generated by elimination of Mo. By applying special preparation conditions, a microstructure composed of martensite, retained austenite and a fine network of special carbides was obtained already in the as-cast state. This material exhibits extremely high compression strength of over 5000 MPa combined with large compression strain of more than 25 % due to deformation-induced martensite formation. With this alloy a new class of TRIP assisted steels was found, which shows an extreme mechanical loading capacity.

5:10 PM
Accounting for High Temperature Measurements with Changing Effective Emissivity in PTAW Processing: *Tonya Wolfe*[1]; Hani Henein[1]; [1]University of Alberta

High temperature measurements of PTAW (plasma transferred arc welding) coatings deposited in-situ are required in order to optimize the process. There is wide interest in obtaining high temperature measurements for other high temperature processes using infrared thermography. However, the reliability of the quantitative data is often in question. Changes in emissivity with temperature, surface condition and phase change challenge the credibility of infrared results. In this paper, the methodology developed and applied to PTAW in order to generate reliable temperature measurements of the surface of the deposit upon cooling after the arc is extinguished, will be described. The methodology applies the coupled use of differential scanning calorimetry, laser reflectance pyrometry, infrared thermography and mathematical modeling.

5:30 PM
The Role of Microtexture on Fatigue Lifetime Variability and Crack Initiation Mechanisms: *Christopher Szczepanski*[1]; James Larsen[2]; Lee Semiatin[2]; [1]UTC/AFRL; [2]AFRL

Microtexture is known to affect the fatigue behavior of alpha + beta titanium alloys as numerous studies have cited microtextured regions as the fatigue crack initiation sites. To quantify the effect of microtexture on the fatigue behavior of alpha + beta titanium alloys, three different microstructural conditions of TI-6Al-4V have been produced via distinct thermomechanical processing routes: a duplex microstructure containing microtexture, a beta annealed structure containing microtexture and a duplex microstructure free of microtexture. The impact of sample orientation on fatigue behavior was examined by testing specimens along three different orientations relative to the original plate reference frame; RD, TD, and 45° from the RD. The mechanism of fatigue crack initiation will be discussed with regard to microstructural condition (processing history) and sample orientation. Furthermore, the distributions of fatigue lifetimes will be characterized based on processing condition to determine if the presence of microtexture significantly impacts fatigue lifetime variability.

Recycling General Sessions: Waste Utilization

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division, TMS Light Metals Division, TMS: Recycling and Environmental Technologies Committee
Program Organizer: Joseph Pomykala, Argonne National Laboratory

Wednesday PM — Room: 206
February 17, 2010 — Location: Washington State Convention Center

Session Chair: Jeffrey Spangenberger, Argonne National Laboratory

2:00 PM
Analysis of Light Hydrocarbon Gases in the Pyrolysis and Combustion Processes of Waste Tires: *Joner Alves*[1]; Chuanwei Zhuo[2]; Yiannis Levendis[2]; Jorge Tenorio[1]; [1]University of Sao Paulo; [2]Northeastern University

The disposal of scrap tires has been a serious environmental problem. The treatment of this waste by pyrolysis and combustion has advantages as landfill releasing and a production of fuel. However, that processes needs a rigid control of emissions. This work presents a study of the light hydrocarbon gases (HC) generated during the burn of waste tire chips in a two-stage laminar-flow horizontal furnace. Different temperatures in the primary and secondary stage of the furnace were tested, was also varied the oxygen/nitrogen percentage during the combustion process. A Gas Chromatograph (Agilent 6890 Series GC-FID/TCD system) was used to separate and characterize the components of the gases mixture. The results showed the behavior of the gases during the burn of tires, providing valuable information to the control of hydrocarbon emissions.

2:25 PM
Utilization of Brazilian Waste Mica in Preparation of Pigments: *Shirleny Santos*[1]; Silvia Cristina França[2]; Tsuneharu Ogasawara[3]; [1]COPPE/UFRJ/CETEM; [2]CETEM; [3]COPPE/UFRJ

Muscovite mica crystals lower than 15 mm diameter are discarded as "trash mica" in the mining area in Borborema-Seridó (BRAZIL). This work has the objective of ore dressing and purifying the "trash mica" aimed use it at preparation of pearlescent pigment. The muscovite was dry ground using knives mills and an ultrasound treatment. It was possible to achieve 67% of mica with particle size lower than 100 µm. This product was used in the preparation of brilliant pigments based on muscovite flakes covered with rare earths oxides (CeO2, PrO2, Ce0,95Pr0,05O2). The pigments were characterized by X-ray Diffraction, Thermal analysis and scanning electronic microscopy. The color of the resulting pigments was analyzed using the CIELAB method and it has showed the following colors: muscovite-CeO2 – yellow, muscovite-PrO2– black and muscovite-Ce0,95Pr0,05O2 – orange. Those results have shown that the "trash mica" is suitable for use in the preparation of pigments.

2:50 PM
Effect of Processes in Degraded Decoloration of Frying Oil Treated with Brazilian Clays: Elaine Araújo[1]; *Edcleide Maria Araújo*[1]; Marcus Vinícius Lia Fook[1]; Sara Verusca de Oliveira[1]; Divânia Ferreira Da Silva[1]; Dayanne Diniz De Souza[1]; [1]Federal University of Campina Grande-UFCG

The process of developing frying characteristics of odor, flavor, color and texture those make the food more attractive to the consumer. During this process, termooxidativas changes occur that alter the quality of oil. Three agents contribute to compromising the quality and modify the structure of frying oil subjected to different temperatures: the humidity, the oxygen and causes to oxidative modification. The oil when frying suffers oxidation process tends to darken, increase the viscosity, increase the formation of foams and develop undesirable flavor and aroma. The aim of this study, through the techniques of kinematic viscosity and acidity content of the effect of bleaching clays Brazilian oil for frying that went through different processes of degraded frying oil treated with Brazilian clays. The results showed that the oils subjected to higher temperatures rose a greater time to clear when compared with those submitted to low temperatures.

3:15 PM
Reuse of Fired Red Ceramic Brick Waste: *Carlos Maurício Vieira*[1]; Sergio Monteiro[1]; [1]State University of the North Fluminense

In the county of Campos dos Goytacazes, north of the State of Rio de Janeiro, Brazil, there is a large production of red ceramic, mainly perforated bricks. A percentage of these bricks are damaged during the firing processing and become a red ceramic waste. This work investigates a possible solution to this environmental problem through the mixture of fired brick wastes, up to 20 wt.%, with clay bodies to produce red ceramics. Body samples were initially tested for plasticity by the Atterberg limits. Cylindrical pressed bodies were fired at temperatures varying from 500 to 1100ºC. After firing, samples were then tested for linear shrinkage, water absorption and mechanical strength. The results showed that brick waste addition did not changed the workability of the clay and that up to 5 wt.% of waste no detrimental effect occurred on the fired properties at all temperatures.

3:40 PM
Evaluating the Compressive Strength and Microstructure of Recycled Glass Compacts: *Adele Garkida*[1]; Jiann-Yang Hwang[2]; Xiaodi Huang[2]; Bowen Li[2]; [1]Ahmadu Bello University; [2]Michigan Technological University

Compacts were made using the uniaxial press at 69 MPa from powders of waste drinking glass, fluorescent tubes, laboratory glass and window glass and 5% bentonite as binder. They were sintered at a temperature range of 600°C - 800°C with holding time of two hours. Sufficient fusion of the compacts was established at 700°C. The compressive strengths of these compacts were determined using Instron 4468 Testing Machine. The microstructures of the specimens were observed using a JEOL JSM 820 Scanning Electron Microscope (SEM). The results showed that there was no significant difference in strength among the four types of recycled glass compacts and the maximum compressive strength attained being 61MPa. However the nature of microstructures exhibited incomplete fusion of the glass particles as showed by the presence of pores with irregular shapes. These specimens have come very close to the maximum strength of 69 MPa attainable according to ASTM C 126.

4:05 PM Break

4:20 PM
Preparation of Building Material Using Elemental Sulfur and Heavy-Metal Containing Slag: Yanjie Liang[1]; *Liyuan Chai*[1]; Xiaobo Min[1]; Zhihui Yang[1]; Shaohui Yang[1]; Xi Cao[1]; [1]Central South University

Element sulfur and volatilization kiln slag(VKS)produced by smelter factories were used to produce sulfured building material. The effects of heating mode, material proportion(MS:MWQS), size of waste particles and ratio of aggregate to filler(A/F), on the mechanical properties and leaching toxicities of solidified stuff were investigated. The optimal conditions for the solidification are stepped heating mode, 3:7 ratio of MS to MWQS, particle size less than150μm and 0.15 ratio of A/F. Under the above optimal conditions, the compressive strength of solidified stuff the rises to 35 MPa, and water absorption is up to 4%-6%. Furthermore, when NaOH is applied as an additive in the process of solidification, the concentrations of most heavy metals except Pb2+ have reached the national leaching toxicity standard. The results of X-ray diffraction reveal that sulfured solidification is due to the physical encapsulation rather than chemical transformation.

4:45 PM
Study on the EMD Residue and Shale for Preparing Solidification Brick: Wang Jia[1]; *Peng Bing*[1]; Chai Li Yuan[1]; Zhang Jin Long[1]; Li Guo Liang[1]; [1]Central South University

To employ resource utilization of residue from the electrolytic manganese dioxide(EMD) production, EMD residue combined with shale and fly ash was used as main material to prepare solidification-sintering brick. Compressive strength and leaching toxicity were chosen as main indexes and then the effect of sintering temperature, sintering time, solid waste ratio and cooling process on its mechanical strength and heavy metal solidification effect was studied. Calcined residue had capability of solidifying heavy metal. By optimizing preparation process, with EMD residue proportion no more than 40% the sample brick treated at T=1073~1273K for 3~5h, then cooled by 873K-semi-quench exhibited good performance and accorded with the national standard.

5:10 PM
Experimental Study on the EMD Residue Admixture Cementitious Material: Wang Jia[1]; *Peng Bing*[1]; Chai Li Yuan[1]; Zhang Jin Long[1]; Li Guo Liang[1]; [1]Central South University

To employ resource utilization of residue from the electrolytic manganese dioxide(EMD) production. As a substitute for partial gypsum, EMD residue combined with fly ash was added into cement clinker to prepare EMD residue admixture cementitious material. Compressive strength and leaching toxicity were chosen as main indexes in addition to XRD analysis, orthogonal analysis and SEM analysis. The effect of activation means, solid waste ratio, water-cement ratio and maintenance means on its mechanical strength and heavy metal solidification effect was studied. The residue treated by calcination, mechanical-activation and sulphate-activation exhibited good cementing performance. By optimizing preparation process, the sample prepared at residue: gypsum: fly-ash=1:1:1, water-cement ratio=0.3 and maintained at 293k in constant temperature and humidity equipment for 1 day and then in air for 6 days accorded with the slay cement national standard.

5:35 PM
Study of Recycling Aggregates of Concrete Waste in Pervious Concrete: *Prakash Parasivamurthy*[1]; KiranKumar BV[1]; Veena Jawali[2]; [1]Dayanada Sagar College of Engineering; [2]B.M.S.College of Engineering

Paper aims to study the Recycling of aggregates of concrete waste (CW) in pervious concrete. The size of the aggregate and the proportion of the particles in the coarse aggregate on the properties of the pervious concrete are investigated. The work includes, type, testing and evaluating quality of aggregate made from CW and evaluating effect of replacement of natural aggregate by recycled aggregate in Pervious concrete. The 28-day strength of CW used pervious concrete was about 3% to 11% lower than that of the pervious concrete made of natural aggregate . The infiltration rate of pervious concrete made of CW fall in the range of 70 to 680 liters per minute per square meter. Pervious concrete made of CW can be used in, pedestrian walkways, nature trials and plazas. It aids in the process of qualifying for LEED Green Building Rating system credits available for using recycled products.

Solid-State Interfaces: Toward an Atomistic-Scale Understanding of Structure, Properties, and Behavior through Theory and Experiment: Thermal, Electrical, and Thermoelectric Behaviors

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS Structural Materials Division, TMS: Chemistry and Physics of Materials Committee
Program Organizers: Michael Demkowicz, Massachusetts Institute of Technology; Douglas Medlin, Sandia National Laboratories; Emmanuelle Marquis, University of Oxford

Wednesday PM — Room: 602
February 17, 2010 — Location: Washington State Convention Center

Session Chair: Srinivasan Srivilliputhur, University of North Texas

2:00 PM Invited
Theoretical and Simulation-Based Predictions of Grain Boundary Kapitza Resistance in Semi-Conductors: *Sylvie Aubry*[1]; Patrick Schelling[2]; Chris Kimmer[3]; Xiaowang Zhou[4]; Reese Jones[4]; [1]Stanford University; [2]University of Central Florida; [3]University of Louisville; [4]Sandia National Laboratories

This talk will present recent theoretical and simulation-based calculations of the thermal conductivity in GaN as well as calculations of the Kapitza conductance in silicon grain boundaries using improved numerical methods such as the direct heat flux, the Green-Kubo and the lattice dynamics methods. A more accurate molecular dynamics calculation of thermal conductivity using the direct heat flux method will be explained and applied to GaN. This method will be compared to the Green-Kubo approach. An improved lattice dynamics approach will also be presented and compared to the direct heat flux method in the case of two different grain boundaries, a low scattering and a high scattering grainboundary in silicon.

2:30 PM Invited
Thermal Conductance of Solid-State Interfaces: *David Cahill*[1]; [1]University of Illinois

Rapid progress in the synthesis and processing of materials with structure on nanometer length scales has created a demand for greater scientific understanding of thermal transport in nanoscale devices, individual nanostructures, and nanostructured materials. In this talk, I will emphasize a critical aspect of this growing field: the thermal conductance of interfaces. We have recently advanced the state-of-the-art of time-domain-thermoreflectance (TDTR) measurements of thermal transport and are using TDTR to study i) heat transport by lattice vibrations across individual interfaces with extremely high and low thermal conductance; ii) interfacial heat transport by electrons in metals; and iii) the thermal conductivity of nanoscale multilayers and disordered layered crystals that violate conventional wisdom about the lower-limit to the thermal conductivity of solids.

3:00 PM
Intrinsic Electric Fields in Nanostructured Oxide Ceramics: Pankaj Nerikar[1]; Christopher Stanek[1]; Susan Sinnott[2]; Simon Phillpot[2]; *Blas Uberuaga*[1]; [1]Los Alamos National Laboratory; [2]University of Florida

Microstructure plays a central role in influencing the properties of materials that determine their performance. Among the many examples of such properties are the nucleation, growth, and subsequent release of fission gases in nuclear fuels, such as urania, UO2. In examining the dependence of fission gas segregation on the structure of symmetric grain boundaries, we have found that, as the spacing between grain boundaries becomes small, an electric field is created across the layers in the ceramic. This field is due to slight distortions in the atomic positions that lead to an asymmetry in the atomic structure. Urania is not unique as other fluorite-structured ceramics also exhibit this field; however, this behavior is not universal. As the bulk of this work relies upon empirical potentials, density functional theory is used to validate the results. We discuss the implications of this field for the structure and behavior of nanostructured ceramics.

3:20 PM
Schottky Barriers at Interfaces between Transition Metals and Strontium Titanate: *Matous Mrovec*[1]; Jan-Michael Albina[1]; Bernd Meyer[2]; Christian Elsaesser[1]; [1]Fraunhofer Institute for Mechanics of Materials; [2]University of Erlangen-Nuernberg

A thorough understanding of interfaces between metals and perovskite oxides is crucial for a successful integration of perovskite materials into modern microelectronic devices. In the case of insulating perovskite oxides, the key feature characterizing the interface is a formation of a potential barrier known as the Schottky barrier. In this work, we present a systematic theoretical study of the Schottky barriers for a series of transition-metal/strontium titanate interfaces. The barriers were calculated using the first-principle mixed-basis pseudopotential method based on density-functional theory. The process of interface formation was analyzed in a step-by-step procedure that enables to distinguish between structural and electronic contributions influencing the Schottky barrier height. This decomposition yields not only detailed information about the most relevant quantities that determine the band lineup at the interface but also provides means to validate fundamental assumptions of phenomenological theories, which estimate the Schottky barrier height from few characteristic material parameters.

3:40 PM
Role of an Interface on the Thermal and Mechanical Characteristics of Heterogeneous Nanocomposites by Correlating Molecular-Quantum Study Focusing on Nanoscale Diffusion and Defect Formation: *Vikas Samvedi*[1]; Vikas Tomar[2]; [1]University of Notre Dame; [2]Purdue University

Interfaces in nanocomposites make available the option to obtain materials with tailored properties by making microstructural changes. In the present research, atomistic analyses of nanocomposite interfaces have been correlated and supported with quantum calculations based on plane-wave basis sets combined with the density function theory (DFT). The focuses of quantum study is on analyzing the nanoscale diffusion phenomena during the formation of interfaces and on correlating the developed understanding with observed thermal and mechanical properties from atomistic calculations. The nanoscale re-configuration at the interfaces leading to the formation of defects and dislocations at high temperatures is studied to predict the overall thermal and mechanical characteristics of such nanocomposites. Analyses of the effect of straining on the nanocomposite property changes are performed to study it as a promising means to obtain nanocomposites with tailored properties.

4:00 PM
Interfacial Defect Mechanism in the Precipitation of Tetradymite Plates in Rocksalt-Structured Tellurides: *Douglas Medlin*[1]; J. Sugar[1]; [1]Sandia National Labs

Controlling the formation and stability of interfaces is important in developing high performance thermoelectric nanocomposites. Here, we consider the transformation mechanism between rocksalt and tetradymite-structured tellurides. Such compounds encompass a wide range of important thermoelectric materials. Our HRTEM observations of tetradymite-structured Sb_2Te_3 plates within rocksalt structured $AgSbTe_2$ have identified a defect that can transform the rocksalt phase to the tetradymite phase through a diffusive-glide mechanism. We analyze this mechanism by establishing the geometric properties of the defect-- namely its step height and Burgers vector, which has components both perpendicular and parallel to the interface. Climb of the perpendicular dislocation component removes a metal plane from the rocksalt phase, forming the tellurium double-layer. Glide of the parallel component places the close-packed planes into the correct tetradymite stacking sequence. The defect properties also give the atomic flux requirements for defect motion, which we analyze for different compositions of the two phases.

Stochastic Methods in Materials Research: Stochastic Methods I: New Algorithms and Model Building

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS/ASM: Computational Materials Science and Engineering Committee
Program Organizers: Richard Hennig, Cornell University; Dallas Trinkle, University of Illinois, Urbana-Champaign

Wednesday PM	Room: 614
February 17, 2010	Location: Washington State Convention Center

Session Chairs: Richard Hennig, Cornell University; Dallas Trinkle, University of Illinois Urbana-Champaign

2:00 PM Invited
Building Effective Models from Sparse but Precise Data: *Axel van de Walle*[1]; Eric Cockayne[2]; [1]Caltech; [2]NIST

A common approach in materials science is the use of a small number of highly accurate but expensive calculations to generate data to fit the parameters of a less accurate but more computationally tractable ``effective model'' enabling larger-scale simulations. A typical example is the fit of a simplified energy model to accurate quantum mechanical calculations. Although least-squares minimization is traditionally used for this purpose, it is not commonly recognized that this approach implicitly and incorrectly assumes that the uncertainty lies in the data rather than in the effective model. We demonstrate that the fact that the model is less accurate than the data can be properly taken into account within a Bayesian framework. This approach enables a perfect fit to the input noiseless data, while avoiding the usual artifacts of overfitting and enables the seamless inclusion of physical knowledge into the fitting procedure.

2:30 PM
Statistical Learning and Materials Informatics: *Krishna Rajan*[1]; Chang Sun Kong[1]; Prasanna Balachandran[1]; [1]Iowa State University

This presentation explores the application of statistical learning techniques unraveling the complex relationships between structure, bonding and chemistry in inorganic materials – for example, identifying pathways that demonstrate how parameters describing electronic structure, chemistry and crystal geometry "communicate" with each other to ultimately define properties. We show how by integrating electronic and crystal geometry information into both classification and predictive data mining techniques, one can extract complex rule based design strategies for materials. In this presentation we also discuss how statistical learning techniques can be used to augment more classical approaches to computational based design of materials.

2:50 PM Break

3:10 PM Invited
Error Estimation in Density Functional Theory: *Vivien Petzold*[1]; James Sethna[2]; Karsten Jacobsen[1]; [1]Technical University of Denmark; [2]Cornell University

We investigate the use of different statistical approaches for developing new electronic density functionals and for estimating prediction errors of the functionals. The development focuses on generalized gradient functionals with a variable enhancement factor, and the optimization is carried out based on molecular fragmentation energies. The question of overfitting is addressed using bootstrap and the .632 estimator. For the estimation of errors we investigate and compare the use of different model ensembles both using multivariate, regression analysis and other ensembles obtained by optimizing the error prediction. The optimal functional is found to lead to prediction errors considerable smaller than other generalized-gradient functionals and of comparable quality with the computationally much more costly hybrid functionals.

3:40 PM
Applications of Stochastic Geometry for Statistical Representation, Stereological Characterization, Modeling, and Simulations of Material Microstructures: *Arun Gokhale*[1]; [1]Georgia Institute of Technology

Material microstructures are stochastic and three-dimensional (3D), and they usually contain features (particles, grain, voids, etc) that are of complex shapes/morphologies. Statistical spatial correlations often exist among different microstrucutral features and their morphological orientations are not always uniform-random. Stochastic geometry provides a powerful basis for statistical representation, characterization, modeling, and simulations of complex 3D microstructures. This contribution will present applications of stochastic geometry for analytical modeling of triple phase boundaries in the microstructures of solid oxide fuel cell cathodes, stereological characterization of 3D microstructures of liquid phase sintered tungsten heavy alloys from lower dimensional manifolds, statistical representations of microstructures of composites using lineal path probabilities and correlation functions, and computer simulations of realistic 3D microstructures of multi-phase materials.

4:00 PM
Fractal Analysis of Microstructural Images for Evaluation of HSLA Steel: *Mita Tarafder*[1]; I. Chattoraj[1]; S.K. Das[1]; M. Nasipuri[2]; S. Tarafder[1]; [1]National Metallurgical Laboratory; [2]Jadavpur University

Investigation of materials invariably requires usages of high resolution images of material structures for quantification of microstructural features, and subsequent development of correlations with the material properties. Often microstructural images of materials exhibit self similar structures or patterns formed due to network of grain boundaries, presences of precipitates, uneven surface elevations, etc. Microstructural images containing self similar fractal patterns at different length scales or resolutions remain unaffected by translations, rotations, projections and many other operations with regard to images. This makes the fractal analysis a useful technique for quantifying microstructural images by fractal dimension — the non-integer dimensional exponent used for representing non-linear complex phenomena. This paper presents fractal analysis of a set of microstructural images of high strength low alloy (HSLA) steel at various aging conditions and reports that the variation of fractal dimensions identifies the morphological changes occurring in nano-scale due to copper precipitation.

4:20 PM Break

4:40 PM
Two Stochastic Mean-Field Polycrystal Plasticity Methods: *Michael Tonks*[1]; John Bingert[2]; Curt Bronkhorst[2]; Daniel Tortorelli[3]; [1]Idaho National Laboratory; [2]LANL; [3]University of Illinois at Urbana-Champaign

Mean-field polycrystal plasticity methods efficiently determine the resultant stress and texture evolution due to an applied strain. However, the deformation of the individual crystals must be approximated since the crystal topology is not represented. In this work, we develop two models in which the crystal deformations are approximated stochastically. Through comprehensive CPFEM analyses of an idealized tantalum polycrystal, we verify that the velocity gradients tend to follow a normal distribution and surmise that this is due to the crystal interactions. We draw on these results to develop the stochastic Taylor model (STM) and the stochastic no-constraints model (SNCM), which differ in the manner in which the crystal strain rates are prescribed. Calibration and validation of the models are performed using data from tantalum compression experiments. Both models predict the compression textures more accurately than the fully-constrained model (FCM), and the SNCM predicts them more accurately than the STM.

5:00 PM
A Stochastic Continuum Model for Growth and Optimization of Epitaxial Quantum Dot Multilayers: Chandan Kumar[1]; *Lawrence Friedman*[1]; [1]The Pennsylvania State University

Randomly seeded processes at the nanoscale present both challenges and opportunities for materials fabrication. The fabrication of Nanoscale Epitaxial Self-Assembled Quantum Dots (SAQDs) marries stochastic and deterministic influences to produce technologically useful electronic and photonic nanostructures. In this process, strained semiconductor thin films are deposited epitaxially and then spontaneously form quasi-periodic 3D nanostructures. Typical materials systems include Ge_xSi_{1-x}/Si and $In_xGa_{1-x}As$/GaAs. It has been observed that more regularity can be obtained by growing multilayers rather than single films. The fabrication ofSAQD multilayers is modeled as space-time white thermal noise passed through a series of linear and non-linear spatial filters, resulting in a sequence of stochastic partial differential equations that are consistent with thermodynamics. Modeling indicates that this sequence can be tuned to produce more ordered structures by varying spacer layer thicknesses. SAQD multilayer fabrication demonstrate the synergy and competition of stochastic and deterministic effects in nanoscale fabrication.

5:20 PM
Monte Carlo Method for Electromagnetic Scattering Incorporating Finite Element Methods to Generate Scatter Sources for Nanoscale Inclusions in Composites: *Erik Sapper*[1]; Brian Hinderliter[1]; [1]North Dakota State University

Scattering of electromagnetic waves by a composite has a significant impact on its perceived quality, and has been used as a nondestructive measurement surrogate for the health of polymeric composites. Electromagnetic wave scattering is used to estimate flaw size distribution, used as input in calculating fracture failure due to stress concentration. Light scattering from the surface (specular) and reemerging from within a coating (diffuse) is a function of wavelength and the weighted integral of these terms gives the gloss and color of a material, particularly for coatings. Monte Carlo ray tracing is a stochastic computational method used to calculate the transport of electromagnetic waves, with a finite element solution of nanoparticle scattering used to generate a surface source for particles below the geometric limit. A 3-dimensional Monte Carlo/FEA model is being developed, capable of analyzing scattering by composites containing scatterers comparable to or smaller than the wavelength of incident light.

Sustainable Materials Processing and Production: Sustainability in Education

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division, TMS Light Metals Division, TMS: Recycling and Environmental Technologies Committee, TMS: Education Committee
Program Organizers: Christina Meskers, Umicore; Randolph Kirchain, Massachusetts Institute of Technology; Diana A. Lados, Worcester Polytechnic Institute; Markus Reuter, Ausmelt Limited

Wednesday PM — Room: 2B
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Diana Lados, Worcester Polytechnic Institute; Adam Powell, Opennovation

2:00 PM Introductory Comments

2:05 PM Invited
Appropriate Technology and Sustainability: *Richard LeSar*[1]; [1]Iowa State University

Sustainability will require more from engineering than the development of technology or structures. Engineering must also take into account the effects of that technology on the integrated social, economic, and environmental processes that constitute our society. Schumacher introduced the powerful concept of an appropriate technology, by which he meant a technology that is appropriate to the environmental, educational, cultural, and economic situation for which it is intended. While the principles of appropriate technology have been most commonly applied in the developing world, they are equally valid, and indeed essential, in the developed world as well. In this talk we will review appropriate technology and discuss its applicability in materials development and use. We will end by presenting a strategy for introducing the concepts and applications of appropriate technology in an engineering curriculum.

2:30 PM Invited
Ceramics for Life in Rural Africa: A TMS Grant Update: *Nathan Johnson*[1]; Sara Moser[1]; Andrew Havens[1]; [1]Iowa State University

In 2009, TMS awarded $5,000 to the Iowa State chapters of Materials Advantage and Engineers Without Borders. The collaboration aims to improve the quality of life in Mali by developing clean, safe, and sustainable household technologies that meet basic needs of impoverished families. This grant introduces three technologies into the home: (1) ceramic water filters that remove particulates and bacteria from ground water, (2) materials to construct clean and efficient cooking stoves that reduce indoor air pollution, and (3) bricks to construct houses that do not degrade in the rainy season. A kiln will be constructed in Mali and local artisans trained to support sustainability. The process from scoping the problem, design at Iowa State, and implementation in Mali is a life experience for student engineers to become the leaders that address tomorrow's needs.

2:55 PM Invited
Depth through Breadth: Addressing the Grand Challenges of Teaching Sustainability: *Svetlana Nikitina*[1]; [1]Worcester Polytechnic Institute

While many question "sustainability" as an intellectual field on the grounds that it is too broad and "undisciplined," we are able to achieve a good balance between breadth of coverage and depth of inquiry in our team-taught seminar "The Grand Challenges: Sustainable Development for the 21st Century" offered to first year students at Worcester Polytechnic Institute. We strike this balance between breadth and depth by a) problematizing key sustainability issues in class discussions; b) by explicitly exploring the lenses of different disciplines (the historical context, the scientific facts, the engineering interventions and the philosophical foundations of unsustainable behaviors); and c) by offering our students opportunities to pursue a targeted project on specific sustainability issues (vertical gardening, metals recycling on college campus) through which they gain depth of understanding as well as practical exposure to all components of the problem, which puts them on the path of seeking effective solutions.

3:20 PM
Engagement is an Essential Skill in the 21st Century: Dirk van Zyl[1]; [1]University of British Columbia

As part of the North American regional activities during the Mining, Minerals and Sustainable Development Project (MMSD) one project focused on the development of sustainability evaluations at the operations level. Engagement was identified as one of the seven important questions to be addressed. Engineers and scientists employed in the mining, minerals and materials production arenas must understand the importance of stakeholder engagement, both within and outside the operations as it is essential in the ongoing activities required to contribute to sustainable development. After developing the awareness that a social license can only be contemplated if engagement is in place they also have to develop skills in applying it. This presentation will present the business case for engagement as well as an approach to motivate undergraduate mining engineers to embrace it. The presentation will also review some recent and ongoing research to improve the engagement process.

3:45 PM Break

3:55 PM
Embracing Sustainability in the Materials Engineering Curriculum: Suggestions and Examples to Build Competencies for Today's Materials Engineering Graduate: *Katherine Chen*[1]; Linda Vanasupa[1]; Trevor Harding[1]; Blair London[1]; Richard Savage[1]; [1]Cal Poly State University

To better prepare students for the complex, global challenges of the 21st century, the Materials Engineering department at Cal Poly transformed its curriculum through a NSF-departmental level reform grant to embrace sustainability. While basic principles of materials science and engineering are still at the core, there has been a shift in the approach – from scientific analysis to engineering design with realistic constraints. Central tenets to the new curriculum include systems thinking and the role of engineers in society. These themes are introduced the freshmen year and continue throughout the different years in different courses (e.g., Materials Selection of the Lifecycle). Several courses are now project-based and involve teams of students working on design challenges. Real world contexts and realistic design constraints that involve environmental and societal impacts have provided rich learning experiences for students. Essential professional skills, such as teamwork, communication and project management, are developed in the process.

4:20 PM
Sustainability and Mineral Resource Utilisation: A Study Guide: *William Rankin*[1]; [1]CSIRO Minerals

It is essential that professionals, both technical and non-technical, working in the mineral and metal commodity industries understand the concept of sustainability and its implications for the industry. Undergraduate courses have not done this well in the past. Much has been written in this field, and there have been great advances in understanding. However, much of what has been published is superficial and sometimes misleading, and there is as yet no coherent, single account that can serve as an introduction or overview. This paper presents an outline which can guide readers in developing an understanding of the topic and its relevance to their work. Key references are provided, particularly those accessible on the internet, which will serve to introduce the reader to the important principles and understandings. The guide should also be useful to academics preparing students to work in the minerals and metal production sectors.

4:45 PM Invited
Teaching Design for "Sustainability" on the Basis of Metallurgy and Materials Science: *Markus Reuter*[1]; [1]Ausmelt Limited

Metals play a pivotal role in society as their properties impart unique functionality to engineered structures and consumer products. Furthermore, metals are theoretically infinitely recyclable. However, among others, design complicates recycling due creating complex structures that produce impure recyclates, hence forcing dilution by the use of virgin pure metal. Metallurgical smelting ingenuity, good technology and intelligent use of thermodynamics and transfer processes gets metallurgists a far way down the path of creating high recycling rates; it is however the 2nd Law of Thermodynamics that also flags the limitations of recovering all elements. This is also then directly linked to economics of the various process routes. A key issue is the creation of optimal industrial ecological systems (Web of Materials) that maximize the recovery of materials from ores and recyclates within the boundaries of thermodynamics, technology and economics.

5:10 PM
Materials and Society Resources on the Teaching Archive of the Materials Digital Library: *Adam Powell*[1]; Laura Bartolo[2]; Matthew Krane[3]; Edwin Garcia[3]; Lan Li[2]; [1]Opennovation; [2]Kent State University; [3]Purdue University

MatDL (http://matdl.org) provides stewardship of significant content and services to support the integration of research and education in the materials community. Two of its complementary services are: 1) MatForge (http://matforge.org) and 2) Teaching Archive (http://teaching.matdl.org/), online workspaces for collaborative development of materials simulation/modeling codes as well as core undergraduate materials teaching resources. By offering materials educators convenient access to relevant, shared learning resources based on research, both teaching and learning within materials science and cognate disciplines are positively impacted. This talk will describe MatDL content focused on sustainability. In particular, several of the resources of the Teaching Archive address the issues of sustainability and the impact of materials technology on society.

5:35 PM Concluding Comments

The Vasek Vitek Honorary Symposium on Crystal Defects, Computational Materials Science and Applications: Crystal Defects and Mechanical Properties

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS/ASM: Computational Materials Science and Engineering Committee
Program Organizers: Mo Li, Georgia Institute of Tech; David Srolovitz, Institute for High Performance Computing, Agency for Science, Technology and Research, Singapore; Adrian Sutton, Imperial College London; Vaclav Paidar, Institute of Physics AS CR vvi; Jeff De Hosson, Univ of Groningen

Wednesday PM — Room: 603
February 17, 2010 — Location: Washington State Convention Center

Session Chairs: Ralf Drautz, Ruhr-Universität Bochum; Petros Sofronis, University of Illinois

2:00 PM Invited
Heating Graphene in a Microscope: *Ju Li*[1]; Liang Qi[1]; Li Feng[1]; Jianyu Huang[2]; Ping Lu[2]; Feng Ding[3]; Boris I. Yakobson[3]; [1]University of Pennsylvania; [2]Sandia National Laboratories; [3]Rice University

Curvy nanostructures such as carbon nanotubes and fullerenes have extraordinary properties but are difficult to pick up and assemble into devices after synthesis. We have performed experimental and modeling research into how to construct curvy nanostructures directly integrated on graphene, taking advantage of the fact that graphene bends easily after open edges have been cut on it, which can then fuse with other open edges, like a plumber connecting metal fittings. By applying electrical current heating to few-layer graphene inside an electron microscope, we observed the in situ creation of many interconnected, curved carbon nanostructures, such as graphene bilayer edges (BLEs), aka "fractional nanotubes"; BLE polygons equivalent to "squashed fullerenes" and "anti quantum-dots"; and nanotube-BLE junctions connecting multiple layers of graphene. The BLEs, quite atypical of elemental carbon, have large permanent electric dipoles of 0.87 and 1.14 debye/Å for zigzag and armchair inclinations, respectively. An unusual, weak AA interlayer coupling leads to a twinned double-cone dispersion of the electronic states near the Dirac points. This entails a type of quantum Hall behavior markedly different from what has been observed in graphene-based materials, characterized by a magnetic field-dependent resonance in the Hall conductivity. Further simulations indicate that multiple-layer graphene offers unique opportunities for tailoring carbon-based structures and engineering novel nano-devices with complex topologies.

2:25 PM Invited

Layer Growth by Ion Bombardment: *Miklos Menyhard*[1]; Peter Sule[1]; Janos Labar[1]; [1]Research Institute for Technical Physics and Materials Science

Ion bombardment generally causes the mixing of originally sharp interfaces of imbedded particles bilayers etc. We have found special cases, when the ion bombardment results in layer growth. This strange behavior was explained by the strongly asymmetric material transport induced by the ion bombardment. We could show that applying various ion (30 keV Ga+, 20 keV Ni+) bombardment on Si/Cr and C/Ni bilayers, the transport, induced by the ion bombardment, of Cr and C are order of magnitude larger than those of Si and Ni, respectively. This difference causes layer formations CrSi mixture, and Ni3C and Ni mixture for Si/Cr and C/Ni bilayers, respectively. The newly formed layers join to the reminder matrix by sharp interfaces. We attempted to understand the asymmetric mixing by applying MD simulation. Though a reasonable agreement with the experimental data has been found it has not resulted in an understanding of the phenomenon.

2:50 PM

The Strength and Deformation of Gum Metal: *John Morris*[1]; Eizabeth Withey[1]; Rohini Sankaran[1]; Andrew Minor[1]; Daryl Chrzan[1]; [1]University of California - Berkeley

The name "Gum metal" has been given to a set of ß-Ti alloys that, with appropriate preparation, appear to deform by a dislocation-free mechanism involving elastic instability at the limit of strength. We have studied thei deformation of these materials through instrumented, in situ compression of nanopillars in high resolution TEM. Interesting results include the following: (1) nanopillars approach ideal strength in the limit of small diameter; (2) there is no significant "size effect" in pillar strength until the diameter falls below 100 nm; (3) the deformation mode is fine-scale, even in pillars of 100 nm size, and involves the growth and micro-rotation of ultrafine domains; (4) the dislocations that are imaged in some tests appear pinned by nanobarriers of uncertain nature; (5) a martensitic transformation to the face-centered orthorhombic a" phase is sometimes observed, but is an incidental feature of the deformation rather than a significant cause of it.

3:05 PM

Deformation of Preciptate Platelets in High Strength Aluminum Alloys under High Strain-Rate Compression: K. El-Khodary[1]; William Lee[1]; L. Sun[1]; Bryan Cheeseman[2]; Donald Brenner[1]; *Mohammed Zikry*[1]; [1]North Carolina State University; [2]Army Research Laboratory

The objective of this study is to identify the dominant microstructural and dislocation mechanisms related to the high strength and ductile behavior of high strength aluminum alloys, and how high strain-rate loading conditions would affect the overall behavior. Characterization techniques and specialized microstructurally-based finite-element (FE) analyses based on a dislocation-density based multiple-slip formulation that accounts for an explicit crystallographic and morphological representation of O precipitates and their rational orientation relations was conducted. As the microstructural FE predictions have indicated, and consistent with the experimental observations, the combined effects of different preciptates, acting on different crystallographic orientations, enhance the strength, the ductility, and reduce the susceptibility of 2139-Al to shear strain localization due to dynamic compressive loads.

3:20 PM Break

3:40 PM Invited

Physical and Mechanical Properties of Co3 (Al,W) with the L12 Structure: *Haruyuki Inui*[1]; Norihiko Okamoto[1]; Katsushi Tanaka[1]; Kyosuke Kishida[1]; Takashi Ohashi[1]; [1]Kyoto University

The recent discovery of the stable L12-ordered intermetallic compound, Co3(Al,W) coexisting with the solid-solution based on Co with a fcc structure has opened up a pathway to the development of a new class of high-temperature structural material based on cobalt, 'Co-base superalloys'. However, almost nothing is known about mechanical properties of the constituent L12 phase, Co3(Al,W). We have investigated some physical and mechanical properties of single crystals and polycrystals of Co3(Al,W) with the L12 structure. When judged from the values of Poisson ratio, Cauchy pressure and Gh/Bh, the ductility of Co3(Al,W) is expected to be sufficiently high so that Co3(Al,W) can be used as the constituent phase of 'Co-base superalloys'. The anomalous temperature dependence of yield stress observed above 700°C is attributed to thermally activated cross-slip of a/2<110> dislocations separated by an APB from octahedral to cube slip planes, as observed in many other L12 compounds such as Ni3Al.

4:05 PM Invited

Propagation of Shear Transformation Zone at Sound Velocity in Metallic Glass: *Shin Takeuchi*[1]; Yasushi Kamimura[1]; Takaaki Yoshihara[1]; Keiichi Edagawa[1]; [1]Tokyo University of Science

Molecular dynamics simulation has been performed for a model binary Ni-Y metallic glass produced by melt-quenchng and annealing. The stability of dislocations has been examined by introducing edge and screw dislocations with the Burgers vector of 0.2 and 0.5nm, followed by static relaxation. The stress analysis has shown that the stress field around both edge and screw dislocation center almost completely disappears after relaxation. By applying an initial strain larger than 0.04 to the model, a steady plastic flow occurs only above a critical stress of 0.03*G* (*G*: shear modulus) by forming localized shear transformation zones with a thickness of 1 to 2nm. However, if a dislocation with *b*=0.6nm is introduced at the edge of the model under a stress of 0.026G, a continuous shear band propagation occurs at a high speed of sound velocity, so that the stress field of the moving dislocation is not blunted by relaxation.

4:30 PM Invited

Multiscale Models of Dislocation Core Structures in Iron and Copper: *Nasr Ghoniem*[1]; A. Takahashi[2]; Z. Chen[3]; N. Kioussis[3]; G. Lu[3]; [1]University of California, Los Angeles; [2]Science University of Tokyo; [3]California State University, Northridge

We discuss here a range of multiscale modeling approaches to describe the atomistic structure of dislocation cores in iron. First, we first present a concurrent multiscale approach, where ab initio calculations are directly coupled with MD simulations. Then, we describe a Peirels-Nabbaro sequential multiscale modeling approach that is a hybrid of ab initio and continuum methods for the analysis of dislocation cores in three-dimensional configurations. We also present another approach to describe the core structure of screw dislocations in bcc metals, and that is the hybrid ab initio-based Atomic-Row sequential model. These models are applied to the study of the core strucures in a number of applications in iron: (1) The effect of Cu and Cr Nano-clusters on dislocation cores in α-Fe; (2)Dislocation interactions with nano-scale Y_2O_3 Precipitates; (3) Dislocation-precipitate interaction; (4) DFT Calculations of the effects of stress on Self-Interstitial (SIA) rotation; (5) The structure of SIA clusters in iron and copper; (6) SIA cluster core response to applied shear.

4:55 PM

Quantum Monte Carlo Calculations for Point Defects in Silicon: *Richard Hennig*[1]; W. Parker[2]; K. Driver[2]; J. Wilkins[2]; [1]Cornell University; [2]The Ohio State University

Point defects in silicon have been studied extensively for many years. Nevertheless, there is still no agreement on the formation energies of selfinterstitials in silicon with theoretical predictions and experimental measurements ranging from 2-5 eV. To answer the question of the formation energy of Si interstitials we resort to quantum Monte Carlo (QMC) and hybrid density functional techniques. Previous QMC calculations resulted in formation energies for the interstitials of around 5 eV. We present a careful analysis of all the controlled and uncontrolled approximations that affect the defect formation energies in variational and diffusion Monte Carlo calculations. We find that more accurate trial wave functions for QMC using improved Jastrow expansions and most importantly a backflow transformation for the electron coordinates result in slightly lower interstitial formation energies than previous quantum Monte Carlo calculations in close agreement with hybrid density functional results.

5:10 PM

Modeling of Point Defect Diffusion in Fe-Cr-Ni Alloys Using Ab-initio Based Multi-Scale Approach: *Samrat Choudhury*[1]; Benjamin Swoboda[1]; Leland Barnard[1]; Julie Tucker[2]; Anton Van der Ven[3]; Todd Allen[1]; Dane Morgan[1]; [1]University of Wisconsin, Madison; [2]Knolls Atomic Power Laboratory; [3]University of Michigan - Ann Arbor

Formation and transport of point defects under irradiation are known to play a significant role in determining the temporal evolution of microstructure and structural properties in Fe-Cr-Ni alloys used in nuclear reactors. In particular, radiation induced segregation (RIS) is a process where point defects migrating to sinks leads to changes in composition near sink boundaries. In this work, we calculate diffusion parameters for both vacancy and interstitial mediated diffusion in dilute and concentrated alloys. The phenomenological (L_{ij}) and tracer diffusion coefficients (D*) are calculated based on a multi-frequency approach using ab-initio diffusion energetics for dilute alloys, while a combination of ab initio energetics, cluster expansion formalism and kinetic Monte Carlo approach is used to calculate L_{ij} and D* in concentrated alloys as a function of composition. The diffusion parameters are then used in a rate theory model to predict the evolution of concentration profiles near grain boundaries under irradiation.

5:25 PM

Computing Ab Initio Free Energy Contributions of Point Defects: *Blazej Grabowski*[1]; Lars Ismer[1]; Tilmann Hickel[1]; Jörg Neugebauer[1]; [1]Max-Planck-Institut für Eisenforschung

A common assumption when computing defect concentrations is that the dominant entropy contribution is due to configurational entropy. Other entropy contributions such as harmonic and anharmonic lattice vibrations are assumed to be second order effects and are computationally expensive to calculate. Thus, such contributions have been rarely considered in defect calculations. With the increasing capability of ab initio approaches to e.g. provide accurate free energies to macroscopic approaches (e.g. CALPHAD), the inclusion of the aforementioned smaller entropy contributions will become more and more important. We have therefore developed a hierarchical scheme to coarse grain the configurations space allowing to efficiently calculate harmonic and anharmonic contributions to vacancy formation [PRB 79, 134106 (2009)]. In the present talk we will discuss the application of this approach to vacancies in aluminum.

5:40 PM

Ab Initio Modeling of Dislocation/Solute Interactions in Mg: *Joseph Yasi*[1]; Louis Hector[2]; Dallas Trinkle[1]; [1]University of Illinois at Urbana-Champaign; [2]General Motors Technical Center

New lightweight, strong, formable Mg alloys are of considerable interest to the transportation industries for improved fuel economy. Efficient, accurate computational modeling of dislocations and solute interactions with dislocations is essential for the development of meaningful constitutive models of strength. In magnesium, the basal slip system is the most active. Prismatic dislocations are two orders of magnitude stronger than basal dislocations, but mobility is necessary to achieve the five independent slip systems required for forming. The first principles flexible boundary condition method is used to compute *a*-type screw, edge, and mixed atomic-scale Mg dislocation geometries in the basal slip system as well as *a*-type edge, *c*-type screw and *c*-type edge in the prismatic slip system. For these dislocations, we calculate solute binding energies for many industrially important solutes by direct substitution in the optimized dislocation cores and also from interaction with local slip and strain in the dislocation cores.

5:55 PM

Embrittlement in Metals: An Atomistic Study of the Hydrogen Enhanced Local Plasticity (HELP) Mechanism: *Johann von Pezold*[1]; Liverios Lymperakis[1]; Jörg Neugebauer[1]; [1]Max-Planck-Institut für Eisenforschung GmbH

The embrittlement of metals by H is a long-standing problem, whose underlying mechanisms are still largely unclear. In this study we consider the atomistic basis of the HELP mechanism. According to this mechanism interstitial H shields dislocation-dislocation interactions, resulting in increased dislocation densities and eventually the nucleation of cracks in regions of high H concentrations.Using a combination of density-functional theory calculations, semi-empirical EAM potentials and an effective lattice-gas Hamiltonian we determine the effect of H on the stress field around edge dislocations in fcc metals. Depending on the strength of the H-H interactions, a hydride phase is formed in the vicinity of the dislocation core already at rather modest bulk H concentrations. The formation of this new phase signficantly reduces the shear stress along the glide plane of the dislocation, resulting in reduced separations in dislocation pile-ups and eventually in the onset of localised plastic fracture.

6:10 PM

Atomic Scale Study of the Interaction of Point Defects with Edge and Screw Dislocations in Bcc Iron: *Erin Hayward*[1]; Blas Uberuaga[2]; Chaitanya Deo[1]; Carlos Tome[2]; [1]Georgia Institute of Technology; [2]Los Alamos National Laboratory

Understanding and predicting irradiation creep in structural reactor materials requires a knowledge of physical processes occurring within dislocation cores. Because Linear Elastic theory can not accurately describe core interactions computation with atomistic methods is vital. We perform molecular statics calculations in order to understand the interactions between vacancies and interstitials and line dislocations in bcc iron. These are compared to similar results given by linear elasticity theory. For vacancies and a variety of self-interstitial dumbbell configurations near both edge and screw dislocations, we find significant differences between continuum theory and atomistics. For vacancies some interaction is seen with both edge and screw dislocations where none is predicted. Results for interstitials tended to have a strong dependance on orientation and position about the core. Particularly for the screw, continuum theory misses the tri-fold splitting of the dislocation core which has a large influence on atomistic results.

6:25 PM

Simulation of Tensile Loading of Ag <110> Nanowires with Extremely Slow Strain Rates Using Accelerated Molecular Dynamics: *Chun-Wei Pao*[1]; Danny Perez[2]; Sriram Swaminarayan[2]; Arthur F. Voter[2]; [1]Research Center for Applied Sciences, Academia Sinica; [2]Los Alamos National Laboratory

Nanowires have unique mechanical and electric properties and are very promising for future nanodevices applications. The mechanical properties of these nanowires are of particular interests because they are very different from their bulk counterparts. Atomistic scale simulations such as molecular dynamics (MD) simulation are the best way to characterize the deformation mechanisms of nanowires. However, due to the time scale limitations of MD simulations, the applied strain rates during typical tensile loading simulations are usually tens of millions times higher than those in real world experiments. Here we present our recent study on the simulation of tensile loading of Ag <110> nanowires using massive parallel-replica dynamics simulation. We are able to reach a time scale of 1 ms and extraction velocity of 1 um/s, which corresponds to an approximate strain rate of 400/s at room temperature. We observed a lot of interesting new physics, for the first time, with atomistic resolution. We observed that there exists an optimum strain rate which maximizes the ductility of the Ag nanowire: for strain rates higher or lower than this particular strain rate, the nanowire ruptures at smaller applied strains due to kinetic or thermodynamic reasons. We also observed an interesting self-healing behavior in the Ag nanowire investigated. The stacking faults generated along the axis of the nanowire during tensile loading processes vanished upon further loading due to the passing of another partial slip, which makes the nanowire free of defects again and one atomic plane thinner.

6:40 PM

Modeling of Deformation and Microstructure Evolution in Severe Plastic Deformation: *Hyoung Seop Kim*[1]; [1]POSTECH

The evolution of microstructure and the mechanical properties of severe plastic deformation (SPD) processed materials depend on the plastic deformation behavior during SPD, which is governed mainly by the die geometry, the constitutive behavior of the material itself and the processing conditions. In this study, we describe some of our results of continuum-based modelling and microstructural-based modelling of various SPD processes in order to illustrate the capabilities of the models. Modelling the evolution of microstructural features of misorientation angle using a dislocation cell model during SPD is presented. Of great interest for modelling the effects of SPD on the material microstructure is the misorientation angle distribution using a probabilistic description involving distribution functions in terms of a Fokker-Planck equation derived using the Langevin approach. The dislocation cell model is implemented into the finite element method associated with cellular automata, which show realistic features of evolutions of gain size and misorientation.

The Vasek Vitek Honorary Symposium on Crystal Defects, Computational Materials Science and Applications: Dislocations II

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS/ASM: Computational Materials Science and Engineering Committee
Program Organizers: Mo Li, Georgia Institute of Tech; David Srolovitz, Institute for High Performance Computing, Agency for Science, Technology and Research, Singapore; Adrian Sutton, Imperial College London; Vaclav Paidar, Institute of Physics AS CR vvi; Jeff De Hosson, University of Groningen

Wednesday PM Room: 604
February 17, 2010 Location: Washington State Convention Center

Session Chairs: Christopher Woodward, Air Force Research Laboratory; Ladislas Kubin, CNRS

2:00 PM Invited
Atomic-Scale Modelling of Dislocation Interaction with Nanoscale Obstacles: *David Bacon*[1]; Yuri Osetsky[2]; [1]University of Liverpool; [2]Oak Ridge National Laboratory

Irradiation of metals with high-energy atomic particles creates nanoscale defect clusters that are obstacles to dislocation glide and can give rise to effects such as hardening and strain localisation. Treatment of these effects in the elasticity theory of dislocations is problematic without information about the atomic mechanisms that occur. Atomic-scale computer simulation can provide details of the influence of stress, strain rate and temperature on the mechanisms. Recent results for dislocations gliding under stress against obstacles in a variety of metals across a range of temperature are classified in this presentation. The effects observed vary from reactions in which the dislocation and obstacle are left unchanged, through ones in which the obstacle is changed but the dislocation is not, to ones in which the obstacle is absorbed temporarily or permanently by the dislocation. Although some processes can be represented within the continuum approximation, others cannot.

2:25 PM Invited
Multiscale Models of Dislocation Core Structures in Iron and Copper: *N. M. Ghoniem*[1]; A. Takahashi[2]; Z. Chen[3]; N. Kioussis[3]; G. Lu[3]; [1]University of California, Los Angeles; [2]Science University of Tokyo; [3]California State University, Northridge

We discuss here a range of multiscale modeling approaches to describe the atomistic structure of dislocation cores in iron. First, we first present a concurrent multiscale approach, where ab initio calculations are directly coupled with MD simulations. Then, we describe a Peirels-Nabbaro sequential multiscale modeling approach that is a hybrid of ab initio and continuum methods for the analysis of dislocation cores in three-dimensional configurations. We also present another approach to describe the core structure of screw dislocations in bcc metals, and that is the hybrid ab initio-based Atomic-Row sequential model. These models are applied to the study of the core structures in a number of applications in iron: (1) The effect of Cu and Cr Nano-clusters on dislocation cores in Fi-Fe; (2) Dislocation interactions with nano-scale Y2O3 Precipitates; (3) Dislocation-precipitate interaction; (4) DFT Calculations of the effects of stress on Self-Interstitial (SIA) rotation; (5) The structure of SIA clusters in iron and copper; (6) SIA cluster core response to applied shear.

2:50 PM
Is Dislocation Locking Possible without External Stress?: *Bella Greenberg*[1]; Mike Ivanov[2]; Alexander Patselov[1]; [1]Institute of Metal Physics, Ural Branch, Russian Academy of Sciences; [2]Kurdjumov Institute of Metal Physics, National Academy of Sciences of Ukraine

The theoretically predicted effect of the self-locking of dislocations actually was detected in Ni_3(Al, Nb) and TiAl. By the self-locking we mean transformations of dislocations from glissile to locked configurations at a zero external stress. Experiments included no-load heating after preliminary deformation. Reasons for the self-locking of superdislocations and single dislocations in intermetallics are revealed. By its nature, this process represents the thermally activated flip of a dislocation from a shallow valley to a deep valley of the potential relief. It is the change of the valley depth that stimulates the self-locking of dislocations. The evidences were obtained that the two effects - the anomaly of the yield stress and the self-locking - have the same origin, namely a double-valley potential relief of dislocations. For comparison similar experiments were performed for BCC metals (Armco-Fe and Mo), which have no the σ_y(T) anomaly. The self-locking of dislocations was not observed.

3:05 PM
Brittle–Ductile Behavior and Dislocation Core Structure in Y- and Co-Based B2 Intermetallics: *Oleg Kontsevoi*[1]; Yuri Gornostyrev[2]; Arthur Freeman[1]; [1]Northwestern University; [2]Institute of Metal Physics

Recently, a class of ductile rare-earth B2 intermetallics (such as YCu, YAg, YZn) has been discovered. In addition, high ductility was found in CoZr, belonging to a unique group of Co-based B2 CoX intermetallics (X = Ti, Zr, Hf). We present a systematic investigation of the shear, elastic, and cleavage energetics of Co- and Y-based alloys by means of first-principles FLAPW calculations. We identify that the ductility of Co- and Y-based B2 intermetallics has intrinsic origins and is connected with martensitic instability of B2 phase with respect to B19, B27, or B33 transformation. Using the modified Peierls-Nabarro model with ab initio parametrization we investigate the structure of {001} and {110} dislocations and predict that the <100>{011} dislocations have a wide core and split according to **b** = **b**/2 + **b**/2 scheme. This wil results in a low Peierls stress, high dislocation mobility and easy plastic relaxation leading to high ductility.

3:20 PM Break

3:40 PM Invited
Structure of Random Tilt Boundaries and Dislocation Emission Behavior under Stress: *Diana Farkas*[1]; Laura Patrick[1]; Nicklas Floyd[1]; [1]Virginia Tech

In this talk we will present the results of a large scale atomistic study of tensile deformation in a virtual FCC polycrystalline sample with columnar grain structure, 40 nm average grain size and a [110] texture. The grain boundaries analyzed were all pure tilt with random misorientation angles and crystallographic orientation of the grain boundary plane. We analyzed the structure and energetics of these random boundaries and their response to stress. We will report the details of dislocation emission from the different grain boundaries and relate the process to the structural units present in the boundaries. Finally, we will show how dislocation debris accumulates in the sample and the strain can localize in certain grains and grain regions, driven by the particular local structure and orientation of the various grain boundaries.

4:05 PM Invited
Copper Precipitation Strengthening of Iron and Steels. Dislocation Locking Mediated by Phase Instability: *Yuri Gornostyrev*[1]; [1]Institute of Metalphysics of the Ural Branch of RAS and CJSC Institute of Quantum Materials Science, Ekaterinburg, Russia

The prediction of the mechanical behavior starting from fundamental microscopic physical principles is challenge problem of materials science. The pronounced strengthening effect of copper precipitates in steels has been studied extensively in the past however the mechanism of this phenomenon are still under debate. To make clear the factors controlling the formation of copper inclusions and strengthening we employ a multiscale modeling approach which involves first principles calculations of the effective interaction parameters, subsequent Monte Carlo simulations of Cu precipitation and molecular dynamic simulations of the dislocation – particle interactions. We show that strengthening effect of copper precipitates caused by dislocation locking due to of the phase instability in nanometer-sized bcc Cu-reach precipitates. The experimental features of the mechanical behavior Fe-Cu based alloys are discussed.

4:30 PM
A Peierls Model of Atomic Stick-Slip Frictional Behavior: *Yanfei Gao*[1]; [1]University of Tennessee

In atomic friction measurements, the stick-slip behavior critically depends on lattice structures of the two contacting surfaces, sliding direction, contact size, sliding velocity, environmental temperature, to name a few. By representing the friction as a point mass moving on top of a periodic potential, the Tomlinson approach restricts all the interface atoms to move uniformly, thus unable to explain the effects of lattice incommensurability and many other factors. We attempt to elucidate the atomic-friction mechanisms from the spatiotemporal evolution of interface defects and lattice structure. A Peierls-type framework replaces singular defect model by the inhomogeneous slip field on the interface. Experimental observations, such as structural lubricity, frictional anisotropy, and contact size dependence, can be explained as a consequence of initiation and multiplication of interface dislocations and their interactions with pre-existing interface defects. Drawbacks of the theoretical model are also discussed.

4:45 PM
Atomistic Modeling of Screw Dislocation Mobility in Alpha-Fe: *Neeraj Thirumalai*[1]; Peter Gordon[1]; Ju Li[2]; Youhong Li[1]; Mikhail Mendelev[3]; Michael Luton[1]; [1]ExxonMobil Research and Engineering; [2]University of Pennsylvania; [3]Ames Laboratory

It is well-known that at low temperatures the flow stress in alpha-Fe exhibits strong temperature dependence. This dependence arises from the motion of screw dislocations, known to be controlled by double-kink nucleation. Previous atomistic studies suggested that this temperature sensitivity is partly a consequence of the polarized core structure of the screw dislocations. However, recent ab initio calculations have shown the core structure of screw dislocations to be compact. We have investigated the kink nucleation pathways that control screw dislocation motion using newly developed interatomic potential for alpha-Fe using Nudged Elastic Band (NEB) and Molecular Dynamics (MD) simulations. In addition, we have also investigated the 2D dislocation motion using ab-initio calculations. In this presentation we will discuss the results of this study and its relevance towards understanding low temperature plasticity in alpha-Fe.

5:00 PM
Atomistically Informed 3D Dislocation Dynamics Simulations of BCC Ta: *Z. Wang*[1]; Irene Beyerlein[1]; [1]Los Alamos National Laboratory

Screw dislocations in BCC metals have non-planar cores, which split onto multiple planes and lead to high Peierls stresses. Atomistic simulations find that non-driving stress components affect the core structures and thus change dislocation behavior and macroscopic properties[1]. Our three-dimensional dislocation dynamics simulations of BCC Ta have shown that without proper implementation of fundamental atomistic-level dislocation properties, plastic behavior of single crystals cannot be correctly predicted. The anisotropy of Ta is dependent on the non-driving shear stresses on the {110} slip planes non-parallel to the glide plane of screw dislocations, while its tension/compression asymmetry is dependent on the stress components normal to the Burgers vector. Our work clearly demonstrates the importance of passing atomistic knowledge to models at larger length scales in understanding material behavior.[1]. K. Ito, V. Vitek, "Atomistic study of non-schmid effects in the plastic yielding of bcc metals", Phil. Mag. A, 81:1387-1407, 2001

5:15 PM
Atomistic Investigation and Analysis of Dislocation Precipitate Interactions in Al-Cu Alloys: *Chandra Veer Singh*[1]; Derek Warner[1]; [1]Cornell University

Al-Cu alloys are attractive aerospace materials due to their light weight and strength. The strength of these alloys is primarily controlled by precipitate formation, with the specific type of the precipitate being controlled by the material aging processes. Here we investigate the mechanisms by which a specific and well known class of precipitates, Guinier-Preston (GP) zones, influence plasticity through dislocation interaction. The dislocation-GP zone interaction is found to be either controlled by long range misfit stress fields or short range chemical forces dependent upon the dislocation-GP zone geometry. To best interpret the atomistic simulations in light of experimental literature, we investigate the activation energy barriers for dislocation-GP zone cutting using transition state theory via the finite temperature string method. Specifically, estimates of the yield strength and its rate and temperature dependence extracted from our results are compared to that of underaged Al-Cu alloys.

5:30 PM
Atomistic Simulations of Athermal Cross-Slip at Screw Dislocation Intersections in Face-Centered Cubic Nickel: *Satish Rao*[1]; Dennis Dimiduk[2]; El-Awady Jafaar[3]; Triplicane Parthasarathy[1]; Michael Uchic[2]; Christopher Woodward[2]; [1]UES Inc.; [2]Air Force Research Laboratory; [3]UTC

The Escaig model for thermally activated cross-slip in Face-Centered Cubic (FCC) materials assumes that cross-slip preferentially occurs at obstacles that produce large stress gradients on the Shockley partials of the screw dislocations. However, it is unclear as to the source, identity and concentration of such obstacles in single-phase FCC materials. In this manuscript, we describe embedded atom potential, molecular-statics simulations of screw character dislocation intersections with forest dislocations in FCC Ni to illustrate a new mechanism for cross-slip nucleation. The simulations show how such intersections readily produce cross-slip nuclei and thus are preferential sites for spontaneous athermal cross-slip. The energies of the dislocation intersection cores are determined and it is shown that a partially cross-slipped configuration for the intersections is the most stable. In addition, simple 3-dimensional dislocation dynamics simulations accounting for Shockley partials are shown to qualitatively reproduce the atomistically-determined core structures for the same dislocation intersections.

5:45 PM
Dislocation Statistics in FCC Crystals: *Mamdouh Mohamed*[1]; Jie Deng[1]; Anter El-Azab[1]; [1]Florida State University

This presentation will give an overview of the statistics of dislocations in FCC crystals with the objective of providing closure of the kinetic equations within the framework of density-based models of dislocation dynamics. In this regard, we perform a detailed statistical analysis of dislocation velocity and the resolved shear stress on dislocation segments, and use this analysis to develop a mobility law valid for dislocation density. In addition, we carry out statistical analysis of the spatial and orientation statistics of dislocation and develop analytical correlation formulas suitable for the closure of the kinetic equations governing the density evolution during plastic deformation. The method of dislocation dynamics simulation will be used to conduct numerical simulation of all pertinent statistical measures.

6:00 PM
Modeling of Magnesium <a> and <c+a> Dislocation Cores by First Principles and EAM Potentials: *Thomas Nogaret*[1]; Joseph A. Yasi[2]; Louis Hector Jr[3]; Dallas Trinkle[2]; William Curtin[1]; [1]Brown University; [2]University of Illinois at Urbana-Champaign; [3]General Motors Technical Center

Magnesium has a poor formability due to its HCP structure: < a > dislocations glide easily in the basal planes, but the pyramidal < c + a > and twinning dislocations, that are required to accommodate the deformation along the < c > axis, have high Peierls stresses. The pyramidal deformation modes are not well understood and constitute a great challenge for material scientists. We performed first principles and EAM potential calculations of gamma surfaces and < a > dislocation core properties in basal and prism planes, and the results were compared. One of the tested EAM potentials was found in good agreement with ab-initio calculations and used to study < c+a > dislocations in pyramidal planes. New low energy <c+a> dislocation core structures were observed and their associated Peierls stresses were calculated at 0K and finite temperature.

Thermo-Mechanical Response of Molecular Solids: Multi-Resolution Theory, Simulations, and Experiments: Molecular Solids I

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division
Program Organizers: Alejandro Strachan, Purdue University; Thomas Sewell, University of Missouri-Columbia; Rodolfo Pinal, Purdue University; Chunyu Li, Purdue University

Wednesday PM — Room: 203
February 17, 2010 — Location: Washington State Convention Center

Session Chair: Rodolfo Pinal, Purdue University

2:00 PM Introductory Comments

2:05 PM Invited
Shock-Induced Subgrain Microstructures as Possible Homogenous Sources of Hot Spots and Initiation Sites in Energetic Polycrystals: Julian Rimoli[1]; Ercan Gurses[2]; *Michael Ortiz*[2]; [1]MIT; [2]Caltech

Microscopic defects such as voids are thought to be a prime source of hot-spots in crystalline energetic materials. For instance, the formation of jets during the collapse of voids may result in temperatures and pressures that greatly exceed values in the bulk, thereby promoting molecular decomposition. The impact sensitivity of defect-free energetic single crystals is comparatively less well-understood, but dislocation-mediated plasticity suggests itself as an explanation for the observed orientation dependencies. It is well-known that dislocation-mediated plastic deformation is almost universally inhomogenous at the sub-grain level and exhibits microstructural patterns that include localization of deformation and temperature to slip-lines. We investigate the role of such slip-lines as possible hot-spots for initiation in void-free energetic polycrystals. We account for sub-grain microstructure development by means of an explicit construction that can be shown to be optimal. The construction is integrated into a finite element model to simulate the plate-impact test of PETN.

2:35 PM

Shear-Induced Disordering in Small Molecule Organic Crystalline Solid Materials: Modeling, Characterization and Relevance in Pharmaceutical Drug Products: *Peter Wildfong*[1]; [1]Duquesne University

Small molecule organic crystalline solids and polymers used to manufacture composite solid oral drug products are often subject to phase transitions resulting from exposure to high shear mechanical processing. Transformations to the amorphous state can result in unpredictable product performance. Multivariate logistic regression was applied to a library of 23 organic crystalline materials to develop a model that identifies properties correlating with the potential to become completely disordered upon application of intense mechanical shear. The optimum model combined glass transition temperature and molar volume, which predicted disordering potential in complete agreement with experimental observations. Of the materials studied, theophylline (a common bronchodilator) was observed to be susceptible to significant disordering under shear stress. Compaction of this material alone, and in the presence of common excipients resulted in detectable induction of disorder as evaluated by PDF-transformed PXRD data collected from intact tablets. Implications for drug delivery are discussed.

2:55 PM

Thermo-Mechanical and Spectroscopic (TMS) Analyses of Structural Transformation Produced by Mechanical Processing: Derya Cebeci[1]; Diana Guzman[1]; Dea Herrera[2]; Dor Ben-Amotz[1]; *M. Teresa Carvajal*[1]; [1]Purdue University; [2]Facultad de Farmacia, UAEM

Milling is a method to reduce particle size of materials and it is among the methods used to enhance the dissolution rate and the oral bioavailability of the active pharmaceutical ingredient (API, drugs) with poor aqueous solubility. However, milling brings multiple transformations produced in the API. These transformations and the resulting behavior of certain organic solid materials need a more fundamental understanding.The influence of mechanical stress applied by cryogenic milling of the crystalline organic solids was investigated via thermal, spectroscopic and mechanical analyses. Various model crystalline APIs were cryo- milled followed by characterization using analytical tools such as XRPD, DSC, Raman, DMA and surface analysis by inverse gas chromatography (IGC) to determine the existence of phase transitions phenomena induced during milling. Differences in the behavior between milled, amorphous and crystalline drugs were clearly observed. Selected experimental and theoretical results from this study will be presented and discussed.

3:15 PM

Microstructural Evolution of Molecular Crystals: *Lei Lei*[1]; Marisol Koslowski[1]; [1]Purdue University

Understanding the mechanisms of deformation of molecular crystals is critical in processing of pharmaceutical products as well as in tailoring key drug properties such as dissolution rate and stability. The process of milling of pharmaceutical materials not only results in particle size reduction but also induces a significant degree of disorder in the material. The increase in disorder as a result of milling can be of two types; either crystal lattice defects or amorphous regions. Here we propose a model to study the transition from a high dislocation density crystal to an amorphous material. In particular we analyze the effect of grain and particle size in this transition with 3D dislocation dynamics simulations.

3:35 PM Break

3:55 PM

Mechanical Response of Pharmaceutical and Explosive Molecular Single Crystals: *Kyle Ramos*[1]; Daniel Hooks[1]; David Bahr[2]; [1]Los Alamos National Laboratory; [2]Washington State University

The mechanical response of molecular crystals is important in a variety of applications. Dislocations have been implicated in die compaction affecting the physical integrity and bioavailability of solid dosage pharmaceutical tablets and in initiation mechanisms affecting the sensitivity to detonation of explosives. Nanoindentation investigations of oriented molecular, single crystals have been conducted revealing orientation dependent nucleation of dislocations through load excursion behavior. Atomic force microscopy characterization of the peripheral regions surrounding indentation impressions has allowed direct observation of slip traces and deformation mechanism analysis using zone axis projections. Deformation features indicate the appearance of additional slip modes in terms of cross slip and new slip systems as a function of orientation and indentation load. These observations provide explanations for deformation behavior in terms of compatibility conditions. Experimental data will be presented for exemplary materials from the pharmaceutical and explosive industries.

4:15 PM

Thermal and Elastic Mechanical Properties of Crystalline 1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB): Dmitry Bedrov[1]; Oleg Borodin[1]; Grant Smith[1]; *Thomas Sewell*[2]; Dana Dattelbaum[3]; Lewis Stevens[3]; [1]University of Utah; [2]University of Missouri-Columbia; [3]Los Alamos National Laboratory

TATB is a high-explosive compound that is remarkably insensitive to shock or thermal initiation. Molecular dynamics simulations of TATB crystals were performed using quantum-chemistry-based dipole polarizable and nonpolarizable force fields for hydrostatic pressures up to 10 GPa at 300 K and for temperatures between 200 K and 500 K at atmospheric pressure. The predicted heat of sublimation and room temperature hydrostatic compression curve were found to be in good agreement with available experimental data. The pressure- and temperature-dependent second-order isothermal elastic tensor was determined for temperatures between 200 K and 400 K at normal pressure and for pressures up to 10 GPa on the 300 K isotherm. The results indicate considerable anisotropy in the mechanical response of the triclinic crystal, with modest softening and significant stiffening of the crystal with increased temperature and pressure, respectively. In general, the polarizable potential was found to yield better agreement with available experimental properties.

4:35 PM Invited

Thermodynamic Stability and Formation of Multicomponent Molecular Crystals: Chinmay Maheshwari[1]; Rodolfo Pinal[2]; *Nair Rodriguez-Hornedo*[1]; [1]University of Michigan; [2]Purdue University

Cocrystals offer the advantage of generating solid forms of active pharmaceutical ingredients (APIs) with other molecular components and produce materials with strikingly different and advantageous physicochemical properties such as solubility and stability. Much of the research in this field has focused on the application of supramolecular chemistry concepts to the design of cocrystals while cocrystal formation and structure-property relationships are not well understood. This talk will address phase formation, stability and transformation during the synthesis, processing and use of pharmaceutical cocrystals. A thorough understanding of cocrystal thermodynamics is critical for the development of these materials. Calculation of cocrystal free energies of formation will be presented from thermal analysis of solid phases and solubility behavior of cocrystal and its components.

5:05 PM Invited

Acoustic and Thermal Responses across the Brillouin Zone: *Keith Nelson*[1]; [1]Department of Chemistry, MIT

We have developed time-domain methods for optical generation and measurement of longitudinal and shear acoustic waves spanning much of the Brillouin zone, including MHz-GHz frequencies and micron-nanometer wavelengths. These are being applied to the study of viscoelastic behavior and thermal transport in a wide range of materials. Thermal diffusivity measurements are made directly as well, and the results can be compared to the values determined for wavevector-dependent phonon mean free paths. Finally, we have extended the techniques to permit generation of nonlinear acoustic and shock waves whose propagation and evolution can be observed directly.

Three-Dimensional Materials Science VI: Novel Tools for 3D Data Acquisition and Analysis - Part II

Sponsored by: The Minerals, Metals and Materials Society, ASM International, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, ASM-MSCTS: Texture and Anisotropy Committee, TMS/ASM: Phase Transformations Committee

Program Organizers: Alexis Lewis, Naval Research Laboratory; Anthony Rollett, Carnegie Mellon University; David Rowenhorst, Naval Research Lab; Jeff Simmons, AFRL; Stuart Wright, EDAX Inc-TSL

Wednesday PM Room: 401
February 17, 2010 Location: Washington State Convention Center

Session Chairs: George Spanos, U S Naval Research Laboratory; Nik Chawla, Arizona State University

2:00 PM Invited

X-Ray Synchrotron Tomography for Three Dimensional (3D) Microstructure Visualization and Modeling of Deformation in Metal Matrix Composites: Jason Williams[1]; Anna Tosas[1]; Zeke Flom[1]; *Nik Chawla*[1]; Francesco de Carlo[2]; [1]Arizona State University, School of Mechanical, Aerospace, Chemical, and Materials Engineering; [2]Argonne National Laboratory/Advanced Photon Source

We report on a novel methodology that addresses the critical link between microstructure and deformation behavior, by using a three-dimensional (3D) virtual microstructure as the basis for a robust model to simulate damage caused by deformation. The approach involves capturing the microstructure by novel and sophisticated x-ray tomography techniques, using an x-ray synchrotron source, followed by image analysis, 3D reconstruction of the microstructure, and incorporation into a powerful finite element modeling code for simulation. We will present a case study based on uniaxial tensile deformation of SiC particle reinforced Al alloy matrix composites. In particular, the damage in the form of particle fracture, interfacial debonding, and void growth will be described. Acknowledgment: Use of the Advanced Photon Source was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

2:30 PM

Orientation Determination by Laue Diffractometry in a Robomet.3D System: *Abhijeet Budruk*[1]; Clayton Stein[1]; Marc De Graef[1]; [1]Carnegie Mellon Unversity

There is growing interest in 3D microstructural data across a broad range of length scales. Existing focused ion beam (FIB) scanning electron microscope and micro-miller-optical microscope combinations cannot conveniently provide 3D information for large sample volumes (several cubic millimeters or larger) while simultaneously obtaining orientational data. To this end, a high-resolution x-ray Laue camera has been added to a metallographic Robomet.3D system, a custom integration of off-the-shelf components, including a programmable robot arm, a multiprep polishing machine, a sample preparation stage, and an inverted motorized optical microscope. The combined system will automatically acquire serial sectioning images of microstructures along with orientational information through the automated indexing of x-ray Laue diffraction patterns. In addition to sectioning larger volumes, it has the advantage of acquiring orientational data on ceramic as well as metallic samples, as it does not employ charged particles as in the more conventional FIB+OIM configuration.

2:50 PM

Utilizing the New Femtosecond Laser Tomographic Sectioning Technique: Reconstruction and Analysis of Low Volume Fraction Titanium Nitride Particles: *McLean Echlin*[1]; Naji Husseini[1]; John Nees[1]; Tresa Pollock[1]; [1]University of Michigan

Rarely occurring inclusion phases can determine fundamental material properties, such as fatigue life and shear strength. A titanium-modified 4330 steel system with low volume fraction (0.02 to 0.07%) titanium nitride inclusions was serial sectioned and reconstructed using a recently developed tomographic technique that utilizes a femtosecond laser to perform the machining steps. This sectioning technique operates in a fully automated mode, with fast removal rates of approximately 7.5 x 104 µm3/s, and a minimum slice thicknesses of 50 nm/slice. TiN datasets were collected over unattended 40-48 hour periods, with subsequent segmentation of the image stack taking 3-5 hours. Volume fraction, particle spacing, nearest neighbor distances, and other statistics were compared with mechanically serial sectioned datasets of the same alloy. In Situ spectrographic data collection is also demonstrated as an alternative chemical recognition technique for inclusion phase differentiation.

3:10 PM

Three-Dimensional (3D) Visualization and Modeling of Reflow Porosity in Pb-Free Solder Joints by Lab-Scale X-Ray Tomography: *Ling Jiang*[1]; Martha Dudek[1]; Jason Williams[1]; Nik Chawla[1]; Luke Hunter[2]; S.H. Lau[2]; [1]Arizona State University, School of Mechanical, Aerospace, Chemical, and Materials Engineering; [2]XRadia

X-ray tomography is an excellent non-destructive technique for quantifying microstructures in three dimensions (3D). We have used lab-scale x-ray tomography to visualize the microstructure of a Sn-3.9Ag-0.7Cu/Cu solder joints. The system had a high resolution (1 µm), which was used for visualization of the three-dimensional (3D) characteristics of reflow porosity. The microstructure of the solder joints was visualized using the x-ray microtomography system, followed by monotonic shear and fatigue experiments of theindividual joints. The effect of pore fraction, size, distribution and geometry of each individual joint, was then simulated using the finite element method. A comparison between the experiments and simulations will be discussed.

3:30 PM Break

4:00 PM

Direct Three Dimensional Characterization of Microstructures in a/ß- and ß-Ti Alloys: *Robert Williams*[1]; Daniel Huber[1]; John Sosa[1]; Santhosh Koduri[1]; Vikas Dixit[1]; Peter Collins[1]; Srinivasan Rajagopalan[1]; Hamish Fraser[1]; [1]The Ohio State University

New research tools for the direct 3-D characterization of microstructures have been developed and applied to the characterization of a/ß- and ß-Ti alloys. The first tool can acquire 3-D datasets using various techniques, including: Optical Microscopy (using the RoboMet-3D™), the Dual Beam-FIB (imaging with either secondary or backscattered electrons), 3D EBSD/OIM (for Ti-based alloys), and Energy Filtered (EFTEM) tomography using (scanning) transmission electron microscopy. The second tool provides an "automated" methodology for 3-D reconstructions through image preprocessing on large image stacks, including alignment of individual images, resulting in the reconstruction of microstructural features. The tool provides for isolation of individual features and their refinement when image preprocessing is inaccurate. These tools, and their application to the direct 3-D characterization of microstructures of a/ß- and ß-Ti alloys, will be discussed. Support from the Office of Naval Research and the Defense Advanced Research Agency under contract number N00014-05-1-0504 is gratefully acknowledged.

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3D Characterization, Analysis, and Modeling Tools: *George Spanos*[1]; Andrew Geltmacher[1]; [1]Naval Research Laboratory

The objective of this team project has been to develop a set of tools for the generation, quantitative analysis, visualization, and collaborative exchange of experimental and simulated 3D materials microstructure and properties data. The team consists of eight research groups from various universities and laboratories, including a group at the Naval Research Laboratory (NRL) who assembled the team. The suite of tools developed provides materials researchers and designers with 3D materials data and predictive modeling capabilities, and can be categorized under three components. The first two components include experimental tools for generating and analyzing 3D data, and computational "Evolver" modules for predictive modeling and simulation. The final component is a Web-based 3D Materials Atlas and related materials data environment for interactive exchange of 3D materials data between materials researchers and/or designers. This talk will provide an overview of the program, and outline the individual tasks and team members.

4:40 PM

D3D Design Research Tools: *Greg Olson*[1]; [1]Northwestern University

A suite of tomographic characterization and analysis tools for quantification of the spatial distribution of multiscale particle dispersions has been integrated with a set of high fidelity 3D simulation tools addressing microstructural evolution governing strength, toughness, shear instability resistance and fatigue strength in high-performance steels for naval applications. Atomic-scale LEAP tomographic reconstruction has quantified the obstacle spacing distributions in martensitic steels strengthened by a combination of bcc Cu and M2C carbide precipitation. FIB/SEM reconstruction of a shear band cut from an isothermal shear test specimen taken to the onset of shear localization demonstrates an early stage of microvoid formation at TiC particle clusters. Crack tip reconstruction clarifies the relation of primary voids and the pattern of shear localization that accelerates their coalescence, consistent with multiscale simulations and measured correlation of normalized toughness with critical void growth ratio. ONR/DARPA sponsored.

Ultrafine Grained Materials – Sixth International Symposium: Applications and Transitions

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee, TMS: Nanomechanical Materials Behavior Committee, TMS: Shaping and Forming Committee

Program Organizers: Suveen Mathaudhu, U.S. Army Research Laboratory; Mathias Goeken, University Erlangen--Nürnberg; Terence Langdon, University of Southern California; Terry Lowe, Manhattan Scientifics, Inc.; S. Semiatin, Air Force Research Laboratory; Nobuhiro Tsuji, Kyoto University; Yonghao Zhao, University of California - Davis; Yuntian Zhu, North Carolina State University

Wednesday PM Room: 606
February 17, 2010 Location: Washington State Convention Center

Session Chairs: Suveen Mathaudhu, U.S. Army Research Laboratory; Yuntian Zhu, North Carolina State University; Terry Lowe, Manhattan Scientific; Judson Marte, GE Global Research

2:00 PM Awards Presentation

2:10 PM Panel Discussion

2:30 PM Invited
Can SPD Techniques Provide Bulk Ultrafine Grained Functional Materials?: *Michael Zehetbauer*[1]; [1]University of Vienna

The fact that SPD techniques allow processing of bulk ultrafine grained (UFG) materials with advanced mechanical properties suggests to apply them also for bulk *functional* ones, especially in cases where physical properties could be significantly increased already in UFG materials with small dimensions. Some success has been reached in SPD processed bulk shape memory UFG alloys, UFG metals/alloys for hydrogen storage, and UFG magnetic alloys. However, applying SPD for achieving bulk UFG materials with other functional properties like thermoelectric ones, or like such being tunable by electronic interface charging, seems questionable. Alternative processing routes using SPD for consolidation of powder UFG materials from ball milling and other techniques may open some chances here.

2:50 PM
Corrosion and Mechanical Properties of a Steel Processed by SMAT in Contrast to Its Coarse Grained Counterpart: *Indranil Roy*[1]; Christian Wilkinson[1]; Rashmi Bhavsar[1]; Jian Lu[2]; Yuntian Zhu[3]; Farghalli Mohamed[4]; [1]Schlumberger; [2]The Hong Kong Polytechnic University; [3]North Carolina State University; [4]University of California, Irvine

Corrosion resistance, the ability of a material to mitigate deterioration of its intrinsic properties due to reactions with its environment, especially in H2S has been an engineering challenge for the oil and gas industry to extract hydrocarbons. Material selection for oilfield tools is generally dictated by a few available standards, for example, NACE MR 01-75. It has been a constant endeavor to develop and qualify more resistant materials for hostile applications that also comply to these standards. In this presentation we discuss the corrosion and salient mechanical properties of a steel treated by SMAT to produce a gradient of nanocrystalline grains on the alloy's surface, starting from a coarse-grained condition.

3:05 PM
Eutectic Structure from an Amorphous Al2O3-ZrO2-Y2O3 System by Rapid-Quenching Technique for Potential Hybrid Solar Cell Application: *Young-Hwan Han*[1]; Jondo Yun[2]; Yohei Harada[3]; Taro Makino[3]; Kwang-Ho Kim[1]; Sehun Kwon[1]; Kazuyuki Kakegawa[3]; [1]Pusan National University; [2]Kyungnam University; [3]Chiba University

Rapid-quenched eutectic crystals are known to be finely oriented, particular microstructures with strong bonding between the component phases, which controls and improves the microstructures. Eutectic ceramics have excellent high temperature strength characteristics, creep resistance, oxidation resistance, and thermal stability at 1700°C in air. Al2O3-based eutectic systems have been studied for use in the emitters of thermophotovoltaic (TPV) generation systems, which emit photons when thermally excited by a heat source.Ternary Al2O3-ZrO2- Y2O3 samples with a eutectic composition were prepared using the rapid-quenching method, with some samples further annealed at 1300°C for 30 min and then slow cooled. The SEM and TEM observations of the ternary samples agreed with the XRD: The rapid-quenched sample was an amorphous phase. Observations showed that the rapid-quenched and annealed sample was completely crystalline with a granular structure and well-defined crystals of 40-60 nm.

3:20 PM Invited
Recycling of Titanium Machining Chips by Severe Plastic Deformation Consolidation: P. Luo[1]; H. Xie[1]; M. Paladugu[2]; S. Palanisamy[2]; M. S. Dargusch[2]; *K. Xia*[1]; [1]University of Melbourne; [2]University of Queensland

It has been demonstrated that SPD can be used to consolidate particles of a wide range of sizes from nano to micro into fully dense bulk material with good mechanical properties. SPD consolidation allows processing to be conducted at much lower temperatures and is therefore suitable for particles with highly metastable structures such as nanocrystalline. It is especially useful in the fabrication of multiphase materials including metal matrix nanocomposites. In this investigation, SPD consolidation was applied to recycle Ti machining chips. In particular, the as-received chips were consolidated by equal channel angular pressing at temperatures between 300 and 600°C with the application of a back pressure from 50 to 200 MPa. Fully dense bulk Ti with ultrafine grain sizes was produced, possessing strength comparable or higher than that of commercially pure wrought Ti. It is concluded that SPD consolidation is a promising method for recycling and value-adding of Ti chips.

3:40 PM
Processing of High Temperature Shape Memory Alloy Ni33.7Ti50.3Pd16 via Equal Channel Angular Extrusion: *Mohammed Haouaoui*[1]; Benat Kockar[2]; Kadri C. Atli[1]; Ji Ma[1]; Ibrahim Karaman[1]; [1]Texas A&M University; [2]Hacettepe University

High temperature shape memory alloys (HTSMAs) with phase transformation temperatures above 100°C have wide uses and opportunities for developments in automotive, aeronautical and oil applications. The main issues in HTSMAs are poor cyclic dimensional stability and fatigue life, and poor formability. Equal channel angular extrusion (ECAE) is used to tackle the plasticity problem in these materials by refining the microstructure and eliminating/breaking up detrimental precipitates. We will present the methodology and the appropriate ECAE processing conditions which permit application of high strains to the hard to work Ni33.7Ti50.3Pd16 material without causing cracking or shear localization of the workpiece. The processing parameters include the canning material, the dimensions of the can, extrusion temperatures, routes and number of passes. Processing Ni33.7Ti50.3Pd16 through route 4E at 425°C proved to increase the dimensional and cyclic stability and decrease the irrecoverable strains. ECAE also increases the fracture toughness by breaking up the brittle precipitates.

3:55 PM
Enabling Near-Net Shaped Forging of Titanium Aerospace Components by Severe Plastic Deformation: *Judson Marte*[1]; Robin Forbes Jones[2]; [1]GE Global Research; [2]ATI Allvac

Severe plastic deformation technologies enable materials capable of low-temperature superplastic response. This presentation will provide an overview of an ongoing collaborative program between ATI Allvac and GE evaluating the production, characterization, and application of ultrafine-grained titanium. Multi-axis forging (MAF) has been used to produce bulk samples with submicron alpha grain size. Extensive characterization of the microstructure shows that, after MAF, the beta phase tends to pin alpha, enhancing thermal stability. Deformation properties have been evaluated and used to make finite element models of near-net shape forging processes. Laboratory-scale near-net shape forgings have been produced to demonstrate feasibility and provide material for microstructural and mechanical evaluation, which will also be presented.

4:10 PM Break

4:25 PM Invited

Improved Recrystallized Microstructures in Nb and Ta: *K. Ted Hartwig*[1]; Shreyas Balachandran[1]; Suveen Mathaudhu[2]; [1]Texas A&M University; [2]U.S. Army Research Laboratory

Low temperature superconducting wires are made by extrusion and wire drawing. In all cases, uniform deformation of the wire components is crucial for optimum electrical performance of the wire. Non-uniform deformation of the wire components during fabrication often occurs and can lead to mechanically weak regions, increased electrical resistance, and wire fracture. The origin of nonuniform deformation includes a nonuniform and poorly oriented starting microstructure; a remedy to the problem is microstructural refinement and texture control. Grain refinement and a degree of texture control in recrystallized microstructures can be achieved through uniform, oriented and severe plastic deformation (SPD) allied via multipass equal channel angular extrusion combined with recrystallization annealing treatments. Results from work done on pure niobium and pure tantalum for improved filament and diffusion barrier codeformation behavior in Nb3Sn filamentary superconductors are given to illustrate the benefits of SPD processing for improved microstructures in recrystallized materials.

4:45 PM

Deformation Processing of Nanostructured Alloys and Their Application in the Production of Hollow Structures: *Radik Mulyukov*[1]; Oleg Valiakhmetov[1]; Rafail Galeev[1]; Rinat Safiullin[1]; Aleksey Kruglov[1]; Renat Imayev[1]; Ayrat Nazarov[1]; Victor Ivan'ko[2]; [1]Institute for Metals Superplasticity Problems, Russian Academy of Sciences; [2]CJSC "INNOTEKHPROM"

Principles of production of nanostructured materials by multiple isothermal forging and warm rolling are formulated. The former allows processing of bulk materials with a uniform nanostructure, while the latter transforms these materials into sheet semi-products retaining their nanostructure. On an example of titanium alloys it is demonstrated that technological operations with nanostructured sheet materials such as pressure welding and superplastic forming can be performed at significantly lower temperatures than with sheet materials having conventional fine grains. This opens new possibilities for the fabrication of hollow structures by a combination of pressure welding and superplastic forming. On an example of hollow blades for double-flow aircraft engines the development of a technology for an implementation in the industry is demonstrated. It is shown that the technology proposed provides not only an enhancement of the properties of hollow blades but also makes their production cost, energy and labor effective and ecologically more friendly.

5:00 PM

Design and Realization of High Strength and High Ductility Metallic Nanomaterials: *Jian Lu*[1]; Ai Ying Chen[1]; Hoi Lam Chan[1]; Hong Ning Kou[1]; Lin Li Zhu[1]; Hai Hui Ruan[1]; Ka Po Cheung[1]; [1]The Hong Kong Polytech University

Nanocrystalline materials have attracted considerably scientific interests from both academia and industries due to their unique material properties. We summarize the recent development of the high strength and high ductility metallic nanomaterials. The SMAT(surface mechanical attrition treatment) has been combined with other technologies (co-rolling, electro-deposition, pre- and post- heat treatments) for enhancing the yield stress of the materials by 200% to 300% with limited reduction of elongation. The development of different efficient fabrication methods for obtaining nanomaterials with exceptional high strength and high ductility by different toughening strategies will be presented: layered nanostructured stainless steel, high twin density Cu and Fe based metallic nanomaterials. The results obtained using the multiscale experimental (nanoindentation, in-situ SEM) and simulation (MD, crystal plasticity, multimillions elements FEM) tools for investigating the local mechanical behavior of the graded structural materials will be presented.

5:15 PM Invited

Potential of Severe Plastic Deformation for Producing Bioimplant Materials: *Yuri Estrin*[1]; [1]Monash University

Several techniques of severe plastic deformation (SPD), notably equal-channel angular pressing as a most developed method, are known to lead to extreme grain refinement in metals and alloys. The ensuing improvement of mechanical properties, including enhancement of fatigue strength, opens up possibilities of downsizing metallic bioimplants or using commercial purity materials, such as CP titanium, instead of alloys, thus eliminating the exposure of the patient to toxic alloying elements. Recent studies conducted in a number of research groups suggest that beside the strengthening effect, SPD processing may lead to improved biocompatibility of the prospective implant materials, such as enhanced cell adhesion and accelerated cell growth. An overview of recent developments in this area will be given, with an emphasis on CP titanium for permanent implant applications and magnesium alloys for temporary, bioresorbable implants.

5:35 PM

Concluding Comments