2010 Functional and Structural Nanomaterials: Fabrication, Properties, Applications and Implications: Mechanical Properties 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

Thursday AM Room: 214
February 18, 2010 Location: Washington State Convention Center

Session Chairs: Gregory Thompson, University of Alabama; David Stollberg, Georgia Tech Research Institute

8:30 AM Introductory Comments

8:35 AM
Substrate Effect on the Young's Modulus Measurement of TiO2 Nanoribbons by Nanoindentation: *Xiaoxia Wu*[1]; Terry T. Xu[1]; [1]University of North Carolina Charlotte

Nanoindentation was conducted on individual TiO2 nanoribbons laid on different substrates, including 1 nm thick SiO2 layer on Si, Si(100) and sapphire (0001). The nanoribbons had an average thickness of 30 nm and width of 150 nm. Experiment results showed that substrate has a significant effect on Young's modulus measurement. To further understand the substrate effect, three-dimensional (3D) finite element modeling was carried out to simulate the indentation of nanoribbon-on-substrate systems using the commercial software ABAQUS. Numerical results demonstrated that nanoindentation could measure the intrinsic mechanical properties of the nanoribbon if a suitable substrate was chosen. Otherwise, the Young's modulus of the nanoribbon could be either overestimated or underestimated depending on substrate used. For the TiO2 nanoribbons, the intrinsic mechanical properties could be obtained from the indentation tests when sapphire (0001) was used as the substrate. The Young's modulus of TiO2 nanoribbons was determined to be 375 ± 25 GPa.

8:55 AM
Commercializing Unique Molecular-Scale Surface and Interfacial Coatings: *Eric Bruner*[1]; [1]Aculon, Inc.

Self-Assembled Monolayers of Phosphonates (SAMP) enable a variety of applications by imparting hydrophobicity, adhesion, or corrosion. SAMPs can impart any of these properties as desired to metals, metal oxides and even some polymer surfaces by drawing on a library of structurally tailored phosphonic acids.The secret to the commercialization is covalent bonding, which creates a uniquely strong attachment between the SAMP and substrate. The SAMP is one approximately 1.5 nm thick. It completely covers the material to which it is applied, and assures total surface coverage regardless of the type or texture of that material. The composition of the SAMP determines the properties it imparts to its substrate. Terminal omega group substituents are chosen to act as reactive handles to covalently bond materials subsequently deposited. Using SAMPs as interfacial coating layers is a powerful tool for solving adhesion issues between dissimilar materials.

9:15 AM
Fracture Behavior of Co-Rich Nanocrystalline Soft Magnetic Ribbons: *Maria Daniil*[1]; Paul Ohodnicki[2]; Michael McHenry[2]; Matthew Willard[1]; [1]Naval Research Laboratory; [2]Carnegie Mellon University

(Co,Fe)-based nanocrystalline alloys have good soft magnetic properties at high frequencies and temperatures making them candidates for transformers and inductors. Recently, the fracture toughness of ribbons was found to improve with increased Co-content.In this work, the fracture behavior and mechanical properties of (Co1-xFex)89Zr7B4 (x=0–0.7) nanocrystalline ribbons were studied. These ribbons consist of majority hcp-(Co,Fe) for the Co-rich composition x=0, bcc-(Co,Fe) for moderate and higher Fe contents (x=0.05) and grain sizes below 15 nm for all compositions. The relative strain-at-fracture decreases dramatically for x = 0.15, with corresponding brittle fracture surfaces, no shear banding and high Vickers hardness values. Samples with lower Fe contents show a maximum strain-at-fracture at x=0.025 and 0.05. The brittle ribbons showed smoother fracture surface, very little or no shear bands and very high hardness. The more ductile ribbons exhibit vein patterned fracture surfaces, significant microvoids, extensive shear bands, and lower hardness.

9:35 AM
Ductility of Bulk Nanostructured Materials: *Yonghao Zhao*[1]; Yuntian Zhu[2]; Enrique Lavernia[1]; [1]University of California-Davis; [2]North Carolina State University

The limited ductility of bulk nanostructured materials has evolved as one of major hurdles limiting widespread application ofthese materials, despite their relatively high strength. The low ductility of bulk nanostructured materials is determined by their limited plasticity and deformation mechanisms. In this talk, we will first review microstructure (including grain size, gain size distribution, grain boundary nature, dislocation density and configuration, texture, solid solute and precipitates)-ductility relationship and external factors (including strain rate, temperature, specimen dimensions, processing artifacts and boundary segregation) that influence the ductility of bulk nanostructured materials, and then summarize effective strategies for improving the poor ductility of bulk nanostructured materials. Finally we will report on recent efforts in our laboratories to implement these strategies in nanostructured Cu, Ni, Ti to obtain both high strength and ductility.

9:55 AM
Evaluation of Fracture Toughness of Carbon Nanotube Reinforced Nano-Aluminum Oxide Via Fractal Approach: *Abhishek Rishabh*[1]; Kantesh Balani[1]; [1]Indian Institute of Technology Kanpur

Aluminum oxide (Al2O3) is considered as high temperature ceramic owing to its high hardness and wear resistance at high temperatures. Lately, the secondary reinforcements, such as of carbon nanotubes (CNTs) have shown to enhance the fracture toughness of Al2O3 matrix by 50% - 300%. The grain size transition from nano to micro of Al2O3 (either equiaxed or elongated), porosity content, and CNT reinforcement can play a major role in dictating the elastic modulus and consequent toughening. Fractal approach has been utilized in the current analytic modeling to predict the fracture toughness of Al2O3-CNT nanocomposites using Mandelbrot fractal geometry with deciding crack pathway. This new approach of considering circumferential crack-path propagation along the CNT surface has shown that experimental fracture toughness values of plasma sprayed Al2O3 – CNT nanocomposites fall within the standard deviation range (or ~2% error) of estimations.

10:15 AM Break

10:30 AM
Warm Sever Plastic Deformation to Form Nanostructured Surface Layer in IF Steels: *Mohammad Nasirizadeh*[1]; Kamran Dehghani[1]; [1]Amirkabir University

Warm sever plastic deformation is introduced in the present work as a new technique to form nanostructure layers on the surface of interstitial free (IF) steels. This technique is an easy, practical, simple and low-cost method to carry out the surface SPD. The process was then modeled using FEM to predict the required strain to attain the nanograins on surface of an interstitial free steel. The results show that at 350°C with the brush rotating of 25000 rpm, one is able to attain a strain about 3.6 required to form nanograins by SPD. The formation of nanograins, 50-150nm, was observed within a surface layer of about 45µm thick. TEM, AFM and SEM techniques were used to characterize the nanostructured layers.

10:50 AM
Bulk Functional Materials Obtained by Shock Waves Compaction of Ultrafine Al and Ti: *Nikoloz Chikhradze*[1]; Constantin Politis[1]; Mikheil Chikhradze[1]; Akaki Gigineishvili[1]; George Oniashvili[1]; [1]Mining Institute/Georgian Technical University

Investigations of shock wave consolidation processes of nano sized Al and ultra-disperse Ti-powder compositions are discussed. The mixtures of ultra-disperse Ti and nano sized (< 50nm) Al powder compositions were consolidated to full or near-full density by explosive-compaction technology. The emulsion and ammonium nitride based industrial explosives were used for generation of shock waves. To form ultra-fine grained bulk TiAl intermetallides with different compositions, ultra-disperse Ti particles were mixed with nano-crystalline

Al. Each reaction mixture was placed in a sealed container and explosively compacted using a normal and cylindrical detonation set-up. Explosive compaction experiments were performed in range of pressure impulse (5-20 GPA). Structural investigations (SEM) and micro-hardness measurements were used to characterize the intermetallides phase composition and mechanical properties. The results of analysis revealing the effects of the compacting conditions and precursor particles sizes, affecting the consolidation and the properties of this new ultra high performance alloys are discussed.

11:10 AM
Corrosion Rates and Mechanical Properties of Nanocrystalline Materials in Contrast to their Coarse Grained Counterparts: *Indranil Roy*[1]; Shehreen Dheda[2]; Manuel Marya[1]; Farghalli Mohamed[2]; [1]Schlumberger; [2]University of California, Irvine

Ultrafine grained (UFG) and nanocrystalline (nc)-metals and alloys are known for frequently outperforming their microcrystalline counterparts due to superior mechanical strengths and wear (abrasion) resistance. The performance of UFG and nc-metals and alloys as bulk material for engineering applications in corrosive environments are however less understood. This paper specifically discusses and compares mechanical and electrochemical properties of nc-nickel, its alloys and UFG Al5083 in contrast to their coarse grained counterparts in various brine environments and temperatures. Weight-loss corrosion and pitting are also discussed in relation to micro/nanostructure and compositions.

11:30 AM
Structural Properties of Nanostructured Fe-Co-V Prepared by Mechanical Alloying and Spark Plasma Sintering: *Baolong Zheng*[1]; Randy Dumas[1]; Asit Biswas[2]; Yizhang Zhou[1]; Kai Liu[1]; Dean Baker[2]; Enrique Lavernia[1]; [1]University of California, Davis; [2]Advanced Powder Solutions, Inc.

FeCo-based soft magnetic materials, having the high saturation magnetization and high Curie temperatures, are ideal for high-temperature applications. Mechanical and magnetic properties of these soft magnetic materials can be further improved by grain size refinement. In this study, nanocrystalline Fe-Co-V soft magnetic alloy powders with an average grain size of 20nm were prepared by severe plastic deformation via high-energy mechanical alloying. XRD analysis showed that bcc-FeCo solid solution was formed after 8 hours of milling. Spark Plasma Sintering (SPS) was used to fabricate bulk nanostructured magnets, whose saturation magnetization, about 229emu/g, is noticeably higher than that of as-milled powders. Characterization techniques including SEM, XRD, DSC, and TEM were used to study the microstructural evolution of both milled powder and SPS consolidated samples under various processing conditions. Magnetic and mechanical properties were measured and further analysis was conducted with emphasis on the relationship among the constitution, processing, microstructure and properties.

11:50 AM
Reticulated Vitreous Carbon Foam Saturated with SiO2 Aerogel for Heat Insulation Purposes: *Liping Shi*[1]; Yesheng Zhong[1]; Xiao dong He[1]; Jia Yu[1]; [1]Harbin Institute of Technology

Reticulated vitreous carbon (RVC) foam has a three-dimensional cellular structure with good thermal insulation and low thermal expansion. Aerogels have lots of particular application especially as superinsulation materials because of their nano-size particles and porous distribution. Silica gels were prepared by taking tetraethoxysiliane (TEOS) as precursor based on two-step acid-base catalysis method and RVC samples were obtained from polyurethane foam impregnated by furfuryl alcohol under different heat treatment temperature. The heat insulation composites, RVC carbon foam matrix impregnated with SiO2 aerogel, were processed by multi-solgel method coupled with dipping treatment. The influence of foam porosity and number of saturated SiO2 aerogel to thermal performance of these composites were investigated by experiments. And the phase composition, microstructure and evolving regularity of this composite were also involved by XRD, EDS and SEM. Besides the mechanical properties and thermal conductivity of carbon foam with and without SiO2 aerogel were compared and discussed.

12:10 PM Concluding Comments

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

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

Thursday AM   Room: 3A
February 18, 2010   Location: Washington State Convention Center

Session Chairs: Magdalena Serrano de Caro, Lawrence Livermore National Laboratory; Joseph Farmer, Lawerence Livermore National Laboratory

8:30 AM Introductory Comments

8:35 AM Invited
Grain Boundary Structure Effects on Radiation Assisted Segregation and Damage: *Zhe Leng*[1]; David Field[1]; [1]Washington State University

Ferritic/martentic steels are attractive materials for use as components in nuclear reactors because of their high strength and good swelling resistance. Grain boundary specific phenomena (such as segregation, voiding, cracking, etc) are prevalent in these materials so grain boundary character is of primary importance. Certain types of boundaries are more susceptible to damage whereas others tend to resist radiation damage. If more damage resistant boundaries can be introduced into the structures, this will result in steel that is more resistant to the processes of degradation that prevail in high-temperature, radiation containing environments. We have characterized the grain boundary structure in HT9 steel by electron backscatter diffraction to identify boundaries that are resistant to degradation and those that are more susceptible to damage in extreme environments. It is found that intergranular damage is mitigated by a high fraction of low energy boundaries due to lower diffusivity and less segregation.

9:05 AM
Materials Behavior under Extreme Conditions: An Aspect from Ab Initio Calculations: *Fei Gao*[1]; H.Y. Xiao[1]; W.J. Weber[1]; [1]Pacific Northwest National Laboratory

SiC and GaN have attracted extensive theoretical and experimental interest due to their potential applications for electronic devices. GaN and SiC are both covalent materials, but with GaN being more ionic and SiC more covalent. SiC is of additional interest because of its potential technological applications in high-temperature structural components for fission and fusion reactors. Recent progress of studying ion-solid interactions in these materials using first-principles approach is reviewed. Large-scale ab initio simulation methods (up to a few thousand atoms) have been developed for the study of ion-solid interactions in materials, and these methods have been employed to investigate defect properties in SiC and GaN. Relative stabilities of these defects have been determined, and their electronic structures provide insight into the configurations and binding properties of these native defects. Atomic structures, formation energies and binding energies of small clusters (both vacancy and interstitial clusters) have been investigated, and their relative stabilities determined. More recently, ab initio molecular dynamics (AIMD) methods have been used to calculate threshold displacement energies and to simulate the primary damage states for the PKA (primary knock-on atom) energies up to 1 keV in SiC and GaN. These simulations provide important insights into electronic effects on ion-solid interaction processes, and reveal that significant charge-transfer occurs between atoms. The charge variation of the recoil atom can decrease the energy barrier for stable defect formation, and the corresponding dynamics evolution is a charge-assisted process, which is expected to have significant effects on defect creation in covalent and ionic materials. Thousand-atom ab initio simulation provides a feasible path to study low-energy ion-solid interaction, charge transfer and charge-redistribution, with first-principle accuracy, in covalent materials. In addition, AIMD methods are used to investigate high-pressure phase transitions in SiC and GaN. These simulations bring a fundamental level of understanding of the wurtzite to rocksalt phase transformation that undergoes inhomogeneous displacements via a tetragonal atomic configuration, and suggest that the transition path may be independent of the presence of d electrons on the cation in GaN. Also the simulated results resolve the discrepancy between experimental observations and theoretical predictions.

9:35 AM

Interatomic Forces in Stainless Steels: *Graeme Ackland*[1]; Derek Hepburn[1]; [1]University of Edinburgh

Stainless steels, primarily FeNiCr based, remain the materials of choice for many reactor components. Modelling of radiation damage at the atomistic level is required to understand the geometry and dynamics of various defects. Molecular dynamics is still the primary method for obtaining such details, and this in turn relies on interatomic potentials.The FeCrC system is uniquely challenging. In addition to the requirement for describing metallic bonding, which is well achieved using Embedded atoms or similar, the energetics depend on antiferromagnetic frustration (FeCR), covalent bonding and charge transfer (carbon). I will describe how appropriate functional forms can be motivated by first principles calculations of relevant configurations. I will then describe how these can be combined with empirical data to provide an optimised parameterization for particular applications. Finally, I will show some applications.

9:55 AM Invited

Thermo-Mechanical Response of a TRISO Fuel Particle in a Fusion/Fission Engine for Incineration of Weapons Grade Plutonium: *Magdalena Serrano de Caro*[1]; P. DeMange[1]; J. Marian[1]; A. Caro[1]; [1]Lawrence Livermore National Laboratory

The Laser Inertial Fusion Engine (LIFE) is an advanced energy concept under development at Lawrence Livermore National Laboratory (LLNL). LIFE is a laser-based inertial confinement fusion engine. This engine could drive a subcritical fission blanket. Different fuel blanket are under consideration which include fertile fuel, such as natural and depleted uranium, or fissile fuel like highly-enriched uranium or weapons-grade plutonium (WGPu). WGPu LIFE is an attractive option because it could achieve a burn up of over 99% fraction of initial metal atoms (FIMAs) in less than 10 years lifetime frame. Materials challenges imposed by the intense pulsed flux of 14MeV neutrons produced by the inertial-confinement fusion (ICF) source, will affect the fuel lifetime. Current LIFE engine designs envisages fuel in pebble bed form with TRISO particles embedded in a graphite matrix, and pebbles flowing in Flibe coolant at T~700C. WGPu LIFE engine operating conditions of high neutron fast fluence, high radiation damage, and high Helium and Hydrogen production pose severe challenges for typical TRISO particles. WGPu LIFE fuel reaches 99.97% FIMA after ~9.4 years after a neutron exposure to fast fluence $F(E > 0.1\ MeV)$ of $\sim 3.62 \times 10^{22}\ n/cm^2$. The thermo-mechanical fuel performance code HUPPCO (High burn-Up fuel Pebble Performance COde) currently under development accounts for spatial and time dependence of the material elastic properties, temperature, and irradiation swelling and creep mechanisms. The effects on the thermo-mechanical response of TRISO particles used for incineration of weapons grade in LIFE engine are analyzed.Preliminary results show the importance of developing reliable high-fidelity models of the performance of these new fuel designs and the need of new experimental data relevant to WGPu LIFE conditions.

10:25 AM

The Evolution and Thermal Recovery of Irradiation Effects in Silicon Carbide: *William J. Weber*[1]; F. Gao[1]; R. Devanathan[1]; Y. Zhang[1]; W. Jiang[1]; [1]Pacific Northwest National Laboratory

Silicon carbide (SiC) is a robust refractory material with potential applications for advanced nuclear energy systems. Experimental and multiscale computational approaches have been integrated to develop fundamental understanding and predictive models of defects, defect production, irradiation damage evolution, and thermal recovery in SiC. In situ ion-beam channeling methods and electron microscopy have been used to study ion-irradiation effects and thermal recovery. Multiscale computation methods have been employed to determine stable defect configurations, defect production, damage efficiency, cascade-overlap effects, close-pair recombination, and defect migration energies and pathways. These studies show that energetic ion-solid interactions in SiC result primarily in the creation of interstitials, vacancies, antisite defects, and small defect clusters that interact to produce long-range structural disorder. The disordering behavior, volume change, and high-resolution images of damage states obtained experimentally and from molecular dynamic (MD) simulations of cascade overlap are in good agreement. This synergistic integration of experimental and computational efforts is providing atomic-level understanding and necessary parameters to model dynamic defect processes and the evolution of irradiation damage in SiC as a function of time, temperature, and dose rate.

10:45 AM Break

10:55 AM Invited

The Synthesis and Sintering of Advanced Fuels: *Brian Jaques*[1]; Daniel Osterberg[1]; Richard Reavis[1]; A. S. Hamdy[1]; Brian Marx[1]; Darryl Butt[1]; [1]Boise State University

The future of nuclear energy in the U.S. and its worldwide expansion depend greatly on our ability to reduce high level waste while maintaining proliferation resistance. Implicit in the so-called advanced fuel cycle is the need for greater fuel burn-up and consequential use of complex nuclear fuels comprised of fissle materials such as Pu, Am, Np, and Cm. Advanced nitride and oxide fuels comprised of ternary and quaternary mixtures of uranium and higher actinides have been considered for applications in advanced nuclear power plants, but there remain many processing challenges. Non- and Low-fertile advanced fuels were synthesized and conventionally sintered in various conditions. The materials were characterized by means of particle size analysis, x-ray diffraction, x-ray photoelectron spectroscopy, electron microscopy, and thermogravimetric techniques.

11:25 AM

Development of a Continuous CVD Process for TRISO Coating of AGR Fuel: *Clay Richardson*[1]; [1]Babcock and Wilcox

As part of the Department of Energy's Advanced Gas Reactor Fuel program, Babcock & Wilcox has developed a fluidized bed chemical vapor deposition process to deposit a TRISO coating on UCO and UO2 kernels. These coated kernels will go into irradiation tests in the Advanced Test Reactor at Idaho National Laboratory. This paper reports on the development activities including the furnace design and the furnace runs made to qualify the coating process.

11:45 AM

Interaction of the Fission Product Pd with TRISO Fuel Coatings: *Yufeng Zhang*[1]; D. Hanks[1]; S. Krause[1]; G. Gajjala[1]; T. Hofmann[1]; L. Weinhardt[1]; M. Bär[1]; C. Heske[1]; [1]Department of Chemistry, University of Nevada, Las Vegas

Tristructural-isotropic (TRISO) nuclear fuel is a key component of high-temperature gas-cooled reactors (HTGR). Typically, SiC is used in the TRISO fuel as the diffusion barrier for both radioactive (fuel) elements and gaseous and metallic fission products, because of its good chemical inertness, high thermal conductivity, and low neutron absorption cross-section. However, it was observed that Pd causes corrosion of the SiC layers in various kernel compositions1, and may lead to coating failure of TRISO fuels. ZrC, a more corrosion-resistant material, is studied as an alternative. Thus, it is important to understand the mechanisms of Pd-SiC and Pd-ZrC interaction. So far, most experiments used bulk-sensitive techniques, which cannot provide direct information about the chemical bonding at the Pd/SiC and Pd/ZrC interfaces. X-ray photoelectron spectroscopy (XPS) is widely used in studying metal-semiconductor interfaces, and has proven to be extremely powerful to understand both the electronic and chemical properties of interfaces and contacts. We will present a detailed XPS study of the formation of Pd/SiC and Pd/ZrC interfaces. The results give direct insight into the local chemical environment of the involved elements (i.e., C, Si, Zr, and Pd at the interface), in particular the formation of secondary phases at the interface.

12:05 PM Invited

ZrC Surface Cleaning and Interaction with the Fission Product Ru: *Stefan Krause*[1]; D. Hanks[1]; Y. Zhang[1]; C. Heske[1]; [1]Department of Chemistry, University of Nevada, Las Vegas

To ensure the safety of TRISO fuel particles, coating layers need to be optimized to encapsulate all fission products in the particle under all possible operating conditions. ZrC is a candidate for a diffusion barrier, and therefore detailed information about the interaction between ZrC and selected fission products is required. We have investigated the surface cleaning of ZrC and the subsequent interface formation with Ru using photoelectron spectroscopy (XPS, UPS), and x-ray absorption as well as emission spectroscopy (XES, XAS). These methods allow the study of changes in the chemical environment of the atoms in the material surface as a function of preparation conditions and Ru deposition. Furthermore, relative surface composition changes can be monitored precisely. We will discuss experiments and procedures to clean the ZrC substrate from oxides, carbon contaminations, and other manufacturing residues. Furthermore, we will present first experiments in which Ru was deposited on ZrC surfaces.

12:35 PM Concluding Comments

Alumina and Bauxite: Alumina Precipitation

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

Thursday AM — Room: 611
February 18, 2010 — Location: Washington State Convention Center

Session Chair: Patrick James, Alumina Partners of Jamaica - Alpart

8:30 AM Introductory Comments

8:40 AM
Study on the Precipitation Kinetics for Improving the Quality of Alumina with Regard to Fines and Attrition Properties: *Narasimharaghavan Krishnaswamy*[1]; Nand Kumar Kshatriya[1]; Supratim Dasgupta[1]; Ramaswamy Jagannathan[1]; [1]Bharat Aluminium Co. Ltd., (A Unit of Vedanta Resources Plc.), BALCO Nagar, Korba

Hydrate of Alumina is precipitated from a super saturated Aluminate liquor, produced from the digestion of Bauxite ores. The two important properties of Alumina which make it qualify as suitable for pre-baked smelter grade are fines (-325 msh fraction) and the Alpha content. Though the second parameter to some extent is dependent on the -325 fraction in hydrate, the growth of the alumina hydroxide is dependent on the size distribution of the seed hydrate present during precipitation and the precipitation conditions. Further the effects of the operating parameters on these product parameters are not welll understood. From this study it has been found that the particle strength is dependent on the precipitation kinetics, the temperature gradient in the precipitators, seed size, seed ratio and the organic contaminants. It could be observed that the product size (-325 fraction) and the strength improved with fine seed addition compared to the coarser seeds.

9:10 AM
Wet Oxidation of Bayer Liquor Organics: Reaction Mechanisms: *Jackie Dong*[1]; James Tardio[1]; Joanne Loh[2]; Greg Power[2]; Chris Vernon[2]; Suresh Bhargava[1]; [1]RMIT University; [2]CSIRO Minerals

Organic impurities in Bayer liquor cause significant losses in productivity and hence the development of improved processes for removing these impurities from this unique solution is of great interest to the alumina industry. Of the various organics removal processes that have been studied and implemented oxidation processes such as wet air oxidation that do not involve the introduction of foreign species into Bayer liquor have received most interest. The chemistry of wet air oxidation of Bayer organics such as sodium malonate and similar compounds is however poorly understood which has hindered improvements in Bayer liquor wet air oxidation processes. In the work reported here results are presented on the influence of key structural features on the reactivity of common Bayer organics under typical wet air oxidation conditions. Reaction mechanisms that occur in the wet air oxidation of several common Bayer impurities are also discussed using 13C NMR and kinetics techniques.

9:40 AM Break

10:00 AM
The Roles of Adsorption in Hydrate Precipitation: *Joanne Loh*[1]; Greta Brodie[1]; Fatima Naim[1]; [1]Parker Centre/CSIRO Light Metals Flagship (CSIRO Minerals)

It has been well established that organic compounds with adjacent hydroxyl groups in Bayer process liquor can inhibit gibbsite precipitation by acting as seed poisons. The degree of inhibition is a function of the number and stereochemistry of the hydroxyl groups. Seed poisons generally adsorb strongly onto hydrate surfaces, implying that surface coverage is the mechanism for yield inhibition. There are examples however of organics that strongly adsorb but do not lead to yield inhibition. There is a possibility that this apparent contradiction may be an artifact of differences in conditions between the adsorption and precipitation experiments. The present work investigates the adsorption and inhibition effects of a range of compounds under strictly similar conditions to clarify the role of adsorption on yield inhibition.

10:30 AM
The Microstructure of Aluminum Hydroxide Powders: *Yu Haiyan*[1]; Li Wencheng[1]; Bi Shiwen[1]; [1]Northeastern University

In this paper, both the foreign and domestic aluminum hydroxide powder products were studied by SEM, XRD, and Raman spectroscopy, and their microscopic structures were also discussed. The results show that the two products are different in three aspects, i.e. the degree of preferential orientation on the(002)crystal plane, the lattice parameters, and the full width at half maximum(FWHM) of Raman peak. The preferential orientation factor, the lattice parameters and the Raman peak FWHM of the domestic product are larger than those of the foreign product. The XRD results indicate that there is no obvious preferential orientation on the (002) crystal plane of the foreign product. The foreign product rather shows preferential growth on a few other crystal planes. Less impurity and defects and better crystallinity possibly contributed to the excellent properties of the foreign product.

Aluminum Reduction Technology: Hall-Héroult Cell: Raw Materials and 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

Thursday AM — Room: 608
February 18, 2010 — Location: Washington State Convention Center

Session Chair: Charles Mark Read, Bechtel Corporation

8:30 AM Introductory Comments

8:35 AM
Rapid, Non-Destructive Analysis of % Gibbsite in Smelting Grade Alumina: Kerrick Dando[1]; *Neal Dando*[2]; [1]Juniata College; [2]Alcoa

At present, there is no easy-to-use method for performing rapid analysis of gibbsite content in smelting grade alumina (SGA). Such an analysis would help aluminum smelters to distinguish between alumina supplies based on % gibbsite (Al2O3.3H2O), track batch variability and correlate cell performance with SGA quality parameters. This report details the development of a rapid, non-destructive near infrared (NIR) method for the quantitative analysis of weight % gibbsite (Al2O3.3H2O) in smelting grade alumina over the range 0-10 weight %. A sample pre-treatment method was also developed for minimizing the effect of physically adsorbed moisture on the analysis method. The single term linear least squares NIR method developed in this study has a standard error of calibration of 0.27 wt %, a standard error of prediction of 0.50 wt% gibbsite and a method repeatability error (1 standard deviation) of <0.017%.

9:00 AM
Alumina Dissolution Rate as Impacted by Ore Pre-Treatments: *Xiangwen Wang*[1]; Jack Sorensen[1]; Neal Dando[1]; Weizong Xu[2]; [1]Alcoa, Inc.

Alumina dissolution rate in cryolitic electrolytes has been a subject of intensive study over the last several decades. Alumina dissolution rate can be affected by the physical, morphological and microstructural properties of the ore, as well as the dynamic of the feeding process. In this study, alumina ore samples were subjected to treatments under various temperature conditions. The pretreated ore samples were then studied to characterize their overall dissolution rates. The HF release upon immediate ore contact to molten bath was also measured and correlated with ore pretreatment and stage of alumina ore dissolution. Dissolution mechanisms are proposed based on the dissolution rate and observation of morphological/microstructural changes of ore samples and flats/crust formed prior to being dissolved.

9:25 AM
Processing of Anode Cover Material: *Ingo Eick*[1]; Bruno Rausch[1]; Juraj Chmelar[2]; Ulrich Kohaupt[3]; [1]Hydro Aluminium Deutschland GmbH; [2]Hydro Aluminium Metal; [3]Steinert Elektromagnetbau GmbH

For high amperage cell the content and consistency of anode cover material (ACM) is essential for an optimal performance. However, ACM is composed partly from recycled material out of various sources from potroom operation contaminated by impurities. In cooperation with Steinert GmbH an approach was established by Hydro to separate impurities from the ACM stream affecting current efficiency and metal quality. Additionally, repair cost for processing equipment will be reduced and the ACM properties improved.Beside magnetic and eddy current separation an industrial solution for inductive sensor sorting has been examined for different sorting sequences applied to various pre-crushed material. The sorting results are strongly affected by the grain sizes and the sorting sequences of the crushed ACM. In average about 1% aluminium and iron and 2-4% carbon weight percentages were found and separated from the samples which sum to 0.2% current efficiency and 1.3 ppm less iron in metal.

9:50 AM
Statistical Investigation and Modeling of Bath Level in Hall-Héroult Cells: *Jayson Tessier*[1]; Patrice Doiron[1]; [1]Alcoa Deschambault

Industrially, alumina is produced through the decomposition of alumina (Al_2O_3) in metallurgical reactors known as pots. Basically, smelter grade alumina powder has first to be dissolved in an electrolytic bath, which is a molten mixture of cryolithe and fluoride salts. Dissolved alumina is then dissociated to produce aluminium. Bath level control is of great importance to smelter operators as it directly affects different key performance indicators related to current efficiency, energy consumption and metal purity. This paper presents an investigation of the variables having an impact on bath level control. It is presented how pot manipulated and state variables and other parameters are statistically linked to bath levels variations. Moreover, different statistical models are used in order to attempt a prediction and forecast of bath level.

10:15 AM Break

10:25 AM
In Situ Raman Experimental Study of Ionic Species in Cryolite Melts of Various Composition: Sergey Vassiliev[1]; Veronika Laurinavichute[1]; Zoya Kuz'minova[1]; Galina Tsirlina[1]; Evgeny Antipov[1]; *Alexander Gusev*[2]; Dmitry Simakov[2]; [1]Laboratory for Basic Research in Aluminium Production, M.V.Lomonosov Moscow State University; [2]RUSAL

Systematic comparison of Raman spectral behavior for cryolite melts of various cation composition is reported in relation to reactivity of inert anodes for aluminum production.

10:50 AM
In Situ Cell Control: *Michael Schneller*[1]; [1]Consultant

Substituting the pseudo-resistance variable (R_p) with the more statistically robust predicted voltage variable (V_p) can enhance the potline process control tool kit. The predicted voltage variable is able to measure *in situ* bath alumina levels and bath temperatures upon demand. Alumina ore feed rates are based upon the intimate linkage between predicted voltage and bath alumina concentration. Pots are fed ore at a steady state rate to maintain a targeted % Al_2O_3 concentration which decreases the risk of un-dissolved alumina/bath conglomerate formation. Multiple daily bath temperature predictions employing predicted voltage can promote voltage and bath ratio optimization. The Lomb algorithm is used to detect statistically significant voltage cycling as part of a scheme to partition the total pot noise into components: 1) voltage cycling; 2) overvoltage changes; 3) pseudo-white noise. A judicious selection of noise components modify ore feed and voltage decisions.

11:15 AM
Determination of Cryolite Ratio of Aluminum Electrolytes: *Bingliang Gao*[1]; Dan Li[1]; Zhongning Shi[1]; Zhaowen Wang[1]; Bijun Ren[2]; [1]Northeastern University, China; [2]Yichuan Power GroupHead Corporation

In aluminum industry, the molar ratio of sodium fluoride to aluminum fluoride is termed as cryolite ratio. Additives, such as MgF2, LiF, NaCl, KF, were used to improve the properties of electrolyte. However, these additives make the composition of aluminum electrolyte complex, and difficult in accurately determining of cryolite ratio. The purpose of our study is to improve this situation, and makes the determination of cryolite ratio more accurate and practical.XRD that commonly used in industrial smelters has big measurement error and poor reproducibility in determining bath ratio of electrolytes containing additives, such as MgF2, LiF, NaCl and KF. Therefore, the calibration formula for XRD was derived according to the experimental results, and it is believed that it can reduce errors and improve the accuracy of cryolite ratio determination of bath to some extent.

11:40 AM Concluding Comments

Aluminum Rolling: Session I

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee
Program Organizer: Kai Karhausen, Hydro Aluminium Deutschland GmbH

Thursday AM — Room: 615
February 18, 2010 — Location: Washington State Convention Center

Session Chairs: Kai Karhausen, Hydro Aluminium; Gary Parker, Wise Alloys, LLC

8:30 AM Introductory Comments

8:35 AM
Integrated through Process Modeling Using a Virtual Platform for Materials Processing by the Example of a Multi-Pass Rolling Process: *Thomas Henke*[1]; Markus Bambach[1]; Gerhard Hirt[1]; [1]RWTH Aachen University

Material properties are the basis for the functionality of any final product including rolled aluminum products. The material properties depend on the microstructure of the final product. The evolution of microstructure during the whole production chain is greatly influenced by the process parameters (e.g. pass reduction and temperatures). Therefore an extensive through process prediction of materials properties including microstructure is highly important. Such a prediction requires coupling of different models to a virtual process chain starting from a homogeneous, isotropic and stress-free melt and up to the final product, sometimes even beyond.In this paper, we present a new web-based platform – the Aachen virtual platform for Materials Processing (AixViPMaP). This platform combines complex physical material models and application-oriented simulation tools. It comprises a virtual, integrative numerical description of processes and of microstructure evolution along entire production chains. Applications of the platform with respect to hot rolling will be given.

8:55 AM
Aluminium Rolling Simulations Considering Interstep Annealing: *Volker Mohles*[1]; [1]RWTH Aachen University

Intended or unintended annealing in between rolling steps can have a significant impact on the rolling process and the material properties even in cases where no recrystallization but only recovery takes place. To consider this recovery effect in computer simulations, a consistent physical model for the work hardening and recovery during rolling steps and the recovery inbetween is needed. In the simulations presented, the dislocation density based three internal variables model 3IVM+ is used. However, like all statistical flow curve models, 3IVM+ must be calibrated to a set of flow curves. In addition, the recovery parameters of this model need a specialized calibration for the recovery periods. As shown, stress relaxation tests can be used for this. They need a special evaluation, but require rather little experimental effort. The simulations are discussed in respect of their present applicability and aspired future development.

9:15 AM
Grain Interactions and Dislocation Density Evolution during Channel Die Compression of Aluminum: *Alankar Alankar*[1]; Ioannis Mastorakos[1]; David Field[1]; [1]Washington State University

We study the microstructure evolution of a 2D-quasi single layer of large grain aluminum polycrystals using our dislocation density based 3D-crystal plasticity model. Initial grain structure is mapped onto a FEM mesh and the predictions of spatial distribution of plastic microstrain are compared with the experimental work reported in the literature. Evolution of dislocation density, crystallite orientations and the Taylor factor are used to compare the predictions with the experimental observations. Local and non-local both effects are considered and are compared with each other.

9:35 AM
Impact of Solute State and Precipitations on the Properties of 8xxx Alloys after Cold Rolling and Recrystallization: *Galyna Laptyeva*[1]; Carmen Schäfer[2]; Kai F. Karhausen[1]; Volker Mohles[2]; Günter Gottstein[2]; [1]Hydro Aluminium Deutschland GmbH, R&D; [2]Institute of Physical Metallurgy and Metal Physics-RWTH Aachen

The mechanical properties of industrially produced 8xxx cold-rolled sheets and the recrystallization during the subsequent heat treatment are strongly related to the thermal processing and rolling conditions (e.g. rolling speed, pass reductions). Depending on the time-temperature processing conditions (e.g. homogenization schedule) of 8xxx alloys various precipitation states are obtained which can cause a strong hindering up to a complete suppression of the recrystallization. The microchemistry in combination with shear amount are therefore the most important material parameters for the manufacturing of material properties. In this contribution, the interaction of different microchemistry states and softening is modelled. The evolution of solute levels and precipitation is hereby predicted for the respective heat treatment using a precipitation model based on the theory of classical nucleation and growth. The recrystallization is modelled by means of a temporal and spatial resolved cellular automaton. The simulation results are discussed with respect to experimental observations.

9:55 AM Panel Discussion

10:25 AM Break

10:40 AM
Inspection Systems and Data Warehousing of Informaton: *David Pond*[1]; [1]Automation and Control Technology Inc.

As the Aluminum industry continues to face competition and slower economic times, information is needed to improve efficiency, quality and ultimately management control. On the production floor, the task is to make available the information needed to identify issues in the process, enable quality to determine the overall compliance to standards, certify to the customer that the product ordered was produced to their specifications and to do it efficiently with minimal human resource. The data needed to support operations is many times stored throughout the company in different databases. This dispersed data being reported in different formats from different data sources leads to confusion, extensive conversations about data validity, and distracts the organization, preventing it from focusing on other corporate initiatives. A consolidated single warehouse of information will be presented to mitigate this problem.

11:00 AM
Expert5i - Intelligent Software Solution for Yield Optimization along the Production Line of Aluminium Flat Rolled Products: Sigrid Hillebrand[1]; Uwe Knaak[1]; *Reinhard Rinn*[1]; [1]ISRA PARSYTEC GmbH

Surface quality inspection has become state of the art in the production of aluminium flat rolled products. Many production lines in the world for e.g. can end stock, lithographic material, or automotive annealed aluminium are already equipped with surface inspection systems. Inspection systems monitor and document surface defects through the individual coil processing steps, enabling the production managers to react promptly on defects, reduce scrap production, and improve delivered quality. However, surface data alone is not sufficient to optimize processes and production. A huge amount of data at each stage of the aluminium making process is waiting to be utilized for the daily decision making of the production and quality managers. This is how the ISRA Parsytec Enterprise PROduction Management Intelligence software "EPROMI" provides help: It analyzes the available information and generates knowledge-based suggestions for the decision makers to make production and quality decisions and finally ensure yield maximization.

11:20 AM
Possibilities of Laser Meaurement for Aluminum Processing: *Patrick Sonntag*[1]; [1]Nokra GmbH

Effective measurement during processing of aluminum can save cost, time and effort. Implemented in steelworks first, laser measurement is now also applied within aluminum processing lines. Complete dimensions, surface faults, flatness, form faults etc. can be measured at 100% of production within the line. Fault detection before quality control and optimized usage of production equipment can enhance quality, reduce scrap, and lead to a higher percentage of output with required properties. Everything between "width x depth x height" and a complete "virtual piece of metal" is possible, superseding manual measurement and inspection. Usage of laser measurement in steel and aluminum industries has proven the advantageousness of constant, complete, and objective measurement with systems that fulfil the requirements of measurement equipment capability standards. Application of this technology has the potential to enormously save time, cost, energy and additionally enhance quality in metal processing.

11:40 AM Panel Discussion

Biological Materials Science: Computational Materials Science

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

Thursday AM — Room: 205
February 18, 2010 — Location: Washington State Convention Center

Session Chairs: Nima Rahbar, University of Massachusetts Dartmouth; Devesh Misra, University of Louisiana

8:30 AM Invited
Molecular Bioassemblies as Mechanical Systems: *Richard LeSar*[1]; [1]Iowa State University

One of the most intriguing ideas in materials development is to use motor proteins either directly as molecular motors or to provide a means to transport material to desired locations. Modeling and simulation offer a path to increase our understanding of these molecules and, perhaps, to design variations of them that have specific properties. The challenge for modeling and simulation is a familiar one to the materials science community - the length and time scales of importance for the behavior of these molecules span a very large range. At the chemical scale, atomistic simulations are the methods of choice. At the largest scales, one approach is to ignore all atomic-level features and to treat large biomolecules as mechanical systems. In this talk, we will review these mechanical descriptions and discuss an approach to bridge the gap between them and the underlying atomistic nature of the molecules.

9:00 AM Invited
Optimized Design of Porous Titanium for Bio-Medical Applications: Alex Turner[1]; Nikolas Hrabe[1]; *Rajendra Bordia*[1]; [1]University of Washington

Stress-shielding has been recognized as a factor in the reduction of hip implant lifetime. In this presentation, we will discuss the simulated performance of a porous titanium implant with a non-uniform distribution of stiffness. The results are based on a two-dimensional finite element model of an implant-bone system. It was found that implants with high stiffness proximally and decreasing stiffness distally provide significant improvements in bone stimulation (measured in terms of strain energy density) in the proximal regions of the femur relative to a conventional fully-dense Ti implant model and an optimized uniformly porous implant model. These results were then confirmed in bone adaptation simulations that measured bone loss following implantation of the various implant models. Other important issues in the development of gradient porosity structures including processing, and relevant mechanical properties will be discussed.

9:30 AM
Numerical Analysis of Tesselated Shark Cartilage in Bending: Xiaoxi Liu[1]; Mason Dean[1]; Adam Summers[1]; *James Earthman*[1]; [1]University of California, Irvine

A large portion of the skeleton of sharks, skates and rays (Chondrichthyes) is characterized by a tessellated structure, composed of mineralized plates (tesserae) joined by intertesseral ligaments overlaying a soft cartilage core. An understanding of the mechanical advantages provided by this skeletal tissue type has been lacking. An equivalent cross section model was developed to analyze the function of the intertesseral ligaments in regulating the stress distribution within the skeletal tissue during bending. The results indicate that this structure distributes more stress to the tesserae loaded in compression than is distributed to those loaded in tension. This behavior provides plausible advantages for 1) reducing susceptibility to fatigue damage; 2) reducing tearing of the tissue by large tensile stresses and 3) allowing compressive stress to power nutrient flow throughout the unmineralized phase. The present model simulations demonstrate these advantages for a typical geometry and range of ligament properties.

9:50 AM

Binding and Assembly of Material-Specific Peptides on Solid Substrates by Atomic Force Microscopy: *Christopher So*[1]; Megan Noyes[2]; Ersin Oren[1]; Hakim Meskine[3]; Hilal Yazici[4]; Paul Mulheran[3]; Candan Tamerler[4]; John Evans[5]; Mehmet Sarikaya[1]; [1]University of Washington; [2]University of Michigan; [3]University of Strathclyde; [4]Istanbul Technical University; [5]New York University

Understanding biomineralization and the realization of biology-inspired materials technologies depends on understanding the nature of the chemical and physical interactions between proteins and inorganic material surfaces. Here, we combine high-resolution atomic force microscopy (AFM) and nuclear magnetic resonance (NMR) experiments with both atomistic and molecular-scale simulation methods to understand the binding and assembly process of genetically engineered peptides and their correlation with the symmetry of the solid surface lattice. We use several such material-specific binding peptides (BP) in this study including AuBP, GrBP, and MicaBPs onto Au(111), Graphite(0001) and Mica(111) respectively. Through these methods, we identify putative docking sites where surface-exposed residues align with these crystallographic surfaces. Further, using ex situ time-lapsed AFM results we describe the spatial nucleation and growth mechanisms over large timescales by kinetic Monte Carlo (KMC) coarse-grained simulations used to describe inorganic epitaxial processes. Supported by GEMSEC, an NSF-MRSEC, and NSF-BioMat grants at the UW.

Bulk Metallic Glasses VII: Mechanical and Other Properties

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

Thursday AM	Room: 213
February 18, 2010	Location: Washington State Convention Center

Session Chairs: Yanfei Gao, The University of Tennessee; Y. Yokoyama, Institute for Materials Research

8:30 AM Invited

Indentation Creep Behavior of Amorphous Selenium and Amorphous Alloys near the Glass Transition Temperature: *Yanfei Gao*[1]; Caijun Su[1]; George Pharr[1]; [1]University of Tennessee

The indentation response of a creeping solid can be correlated to its uniaxial response, when replacing the uniaxial stress by indentation pressure and the uniaxial strain rate by an effective strain rate. A general definition of the effective strain rate has been provided by using the Hill-Bower similarity transformation method. A stiffness-based methodology has been developed to study the indentation creep behavior at high temperatures. For amorphous selenium, the dependence of stress exponent and activation volume on the temperature and strain rate agrees with the deformation modes in uniaxial compression tests. The decrease of temperature and the increase of strain rate lead to the decrease of activation volume. A similar observation is also found for amorphous alloys. These results are explained from the strain localization behavior in a rate-dependent solid.

8:50 AM

Crystallization Mechanism in Amorphous Cu-Zr System: *Ilkay Kalay*[1]; Eren Kalay[1]; Matthew Kramer[1]; Ralph Napolitano[1]; [1]Iowa State University / Ames Laboratory

The Cu-Zr binary system is the basis for many bulk metallic glass and amorphous crystalline composite materials due to its high glass forming ability. However, the prediction and control of the relative phase stability is elusive because of the complex devitrification behavior of the binary alloy. In this current study, best glass forming compositions in Cu-Zr binary alloy were investigated in terms of crystallization kinetics and thermal stability. The isochronal devitrification phase transformation paths were determined using in situ high energy synchrotron X-ray diffraction (HEXRD) experiments. The transformation kinetics and microstructural evolution during isothermal annealing was investigated using transmission electron microscopy (TEM), HEXRD and differential scanning calorimetry (DSC). The mechanism of crystallization accompanied with TEM at different stages of crystallization and the thermal stabilities will be discussed and compared for best glass forming compositions in Cu-Zr binary alloy system. Research supported by U.S. DOE-OS, Ames Laboratory contract No.DE-AC02-07CH11358.

9:00 AM Invited

Tensile Ductility in Metalic Glass: Z.F. Zhang[1]; F.F. Wu[1]; *Scott Mao*[2]; [1]Shenyang National Laboratory for Materials Science, Institute of Metal Research; [2]University of Pittsburgh

The tensile ductility or brittleness of metallic glasses is strongly dependent on the critical shear offset, which reflects the shear deformation ability of metallic glass. Furthermore, the size effect on the tensile shear deformation of metallic glass can be well understood: with decreasing specimen size smaller than the equivalent critical shear offset, there exists a transition from the unstable shear deformation to the stable shear deformation, which corresponds with the transition from the global brittleness on the millimeter-scale to the large global plasticity and even necking on the millimeter- or sub-millimeter-scale. These results are fundamentally useful to understand the physical nature of tensile shear deformation of various metallic glasses and even to design new metallic glassy materials with good plasticity.

9:20 AM

Crystal Formation at Unusually Low Temperatures: Joachim Bokeloh[1]; Nancy Boucharat[2]; Harald Roesner[1]; *Gerhard Wilde*[1]; [1]University of Muenster; [2]Research Center Karlsruhe

Nanocrystal formation at extremely high number densities is the key reaction that controls the synthesis of high strength nanostructured Al-rich Al-RE-TM (RE: rare earth, TM: transition metal) alloys. With the benefits of increased stability against coarsening and improved mechanical performance at higher nanocrystal number densities, the origin of the nanocrystal formation and the development of methods to tune the microstructure on the nanometer level have been issues of active research and controversial discussions. While previous results clearly indicated the importance of the as-quenched structure of the glass, a correct description of the kinetics of the underlying nucleation and growth processes from the early to the intermediate stages of nanocrystal formation has not been achieved. Recent results from combined measurements by microcalorimetry, modulation calorimetry and quantitative microstructure analyses provide new insight into the early stages of devitrification of Al-rich metallic glasses, indicating the complex processes that proceed during initial crystal formation

9:30 AM Invited

Evolution of Shear Bands in Bulk Metallic Glass Composite: *G. Chen*[1]; J. L. Cheng[1]; H. Bei[2]; C. T. Liu[2]; [1]Nanjing University of Science and Technology; [2]Oak Ridge National Laboratory

The evolution of shear bands in Zr-based bulk metallic glass matrix composite at different tensile strain had been tested under uniaxial tension have been investigated. It is found that on the yield point a few slip bands formed first inside the soft ß-Zr phase.At this time, there are no shear bands being discovered in the glass matrix. As the deformation increases, the density of slip bands in the ß-Zr phase get more. There are shear bands generating from the interface and develop into the glass matrix.The shear bands get more and more till fracture take place.

9:50 AM
Deformation Mechanisms in Amorphous-Crystalline Nanocomposites: *Yvonne Ritter*[1]; Karsten Albe[1]; [1]Technische Universitaet Darmstadt

In order to elucidate the deformation mechanisms present in amorphous-crystalline composites, we have studied different composites consisting of an amorphous Cu_xZr_{1-x} phase and a crystalline Cu phase by molecular dynamics simulations, employing EAM-potentials to model the atomic interactions. Nanolaminates with alternating glass- and crystal-layers serve as model geometries to investigate the properties of amorphous-crystalline interfaces as well as the effect of geometrical confinement. We find the thickness of the individual layers to have a strong influence on the operating deformation mechanisms, both, in the glass and in the crystalline layers.Additionally, shear-banding in the presence of nanocrystalline-precipitates is studied by deforming a fully 3d-sample containing spherical Cu-crystallites in an amorphous Cu-Zr-matrix in tension. Sample dimensions, glass composition and preparation, as well as the loading conditions are chosen to allow for shear band nucleation despite the absence of stress concentrators like pre-existing notches or an indenter-tip.

10:00 AM Break

10:10 AM Invited
Dissimilar Mechanical Properties between Various Families of Bulk Metallic Glasses: *Maria D Baró*[1]; Jordina Fornell[1]; Santiago Suriñach[1]; Weihuo Li[2]; Annett Gebert[3]; Jordi Sort[1]; [1]Universitat Autònoma de Barcelona; [2]Anhui University of Technology; [3]IFW Dresden

The mechanical properties of various families of bulk metallic glasses (BMGs), based on Zr, Ti or rare earths, have been investigated. Although all these alloys share an amorphous structure, their mechanical properties are distinctly different. Namely, while BMGs based on rare-earths fracture before yielding, the Zr-based BMGs show signatures of superplasticity. Moreover, whereas Zr-based and Ti-based BMGs are very hard and exhibit a large Young's modulus, the rare-earth BMGs are relatively soft and show a low Young's modulus. These differences in mechanical behavior can be correlated with the different values of elastic constants and glass transition temperature of the several families of BMGs. Particular emphasis will be given in this presentation to recent results from nanoindentation experiments to shed light on several issues such as the influence of normal stress components acting on the shear plane at yielding, strain rate effects or deformation-induced nanocrystallization.

10:30 AM
Submicron Scale Measurement of Residual-Stress Profiles in Amorphous Materials by the FIB Incremental Slitting Technique: *Bartlomiej Winiarski*[1]; Ali Gholinia[1]; Jiawan Tian[2]; Yoshihiko Yokoyama[3]; Peter Liaw[2]; Philip Withers[1]; [1]University of Manchester; [2]The University of Tennessee; [3]Himeji Institute of Technology

Residual-stresses exist in solids in the absence of external forces or due to thermal gradients, thus alter the component performance and promote/inhibit failure processes. There have been numerous efforts to measure residual-stresses in crystalline, amorphous materials and multilayered coatings (e.g. semiconductor devices, MEMS, nuclear materials) at the micron scale. Diffraction and other conventional laboratory methods are robust to evaluate stresses in crystalline matter, however their application to glassy materials is very difficul and often impossible. We present a new technique for mapping residual-stress profiles in amorphous and crystalline materials with high spatial definition. The new sub-micron-scale mechanical-relaxation method uses FEGSEM-FIB incremental slitting and Digital Image Correlation strain analysis to evaluate residual-stresses in surface-severe-plastic-deformed Zr50Cu40Al10 BMG. The calculation algorithm is based on the Unit Pulse Method and is enriched by Tikhonov regularisation and FEA. We demonstrate that the new technique infers residual-stress profiles in amorphous materials with high spatial definition (200-300nm).

10:40 AM
Heating-Rate-Dependent Crystallization Behavior of a Zr-Based Bulk Metallic Glass: *Hongqing Sun*[1]; Katharine Flores[1]; [1]The Ohio State University

Pronounced asymmetry has been observed in crystallization of multicomponent bulk metallic glasses (BMGs) when they are heated from glassy state versus cooled from the liquid. Understanding the crystallization mechanisms of different heating and cooling conditions is necessary to enable novel processing of BMGs, such as laser deposition or joining. In this work, as-cast $Zr_{58.5}Cu_{15.6}Ni_{12.8}Al_{10.3}Nb_{2.8}$ glass specimens were heated to the melting temperature at heating rates of 0.5 ~ 50 K/s. Lower heating rates resulted in the formation of densely packed nano-scale crystals. TEM and EDS analysis indicates that the nanocrystal nucleation is preceded by phase separation. In contrast, higher heating rates result in the formation of micro-scale spherulites. Nucleation was suppressed by rapid heating, allowing growth to dominate the crystallization process. The rapid transformation from glass to spherulite was accomplished without evidence of prior phase separation. Calculation of crystallization activation energies also indicates various mechanisms at different heating rates.

10:50 AM
Influence of Minor Aluminum Concentration Changes in Zirconium-Based Bulk Metallic Glasses on the Elastic, Anelastic, and Plastic Properties: *Arnaud Caron*[1]; Rainer Wunderlich[1]; Dmitri Louzguine-Luzgin[2]; Guoqiang Xie[2]; Akihisa Inoue[2]; Hans-Jörg Fecht[1]; [1]Institute of Micro- and Nanomaterials, University Ulm; [2]WPI Advanced Institute for Materials Research, Tohoku University

The Poisson's ratio of Zr-based bulk metallic glasses in the System Zr63-xCu24AlxNi10Co3 was found to exhibit a non-monotonous behavior as a function of x when measured with ultrasound by pulse echo technique. Also from wave propagation velocity measurements at different frequencies, i.e. f = 2.25 MHz and f = 10 MHz, a composition dependent anelastic behavior as a function of x is found, exhibiting a similar non-monotonous behavior. In this work we further investigated the plastic deformation and the creep properties of this glass system in compression tests and by nanoindentation. The plastic strain and the measured creep deformation shows correlation with the Poisson's ratio. We then discuss the anelastic behavior observed while measuring the sound wave propagation velocity in the frame of the thermoelastic damping and the bond reorientation as proposed by Egami. Finally we discuss these effects with regards to X-ray diffraction analysis.

11:00 AM
Length Scale Effects on Deformation in a Zr-Based Bulk Metallic Glass: *Ashwini Bharathula*[1]; [1]The Ohio State University

Size effects on plasticity and deformation modes of a Zr-based bulk metallic glass are examined using specimens with diameters ranging from 200 nm – 3.6 µm. Shear banding in micron- and sub-micron-scale testing is more stable than in macro-scale testing because of the smaller ratio of the specimen to load frame stiffness. As the specimen size decreases, smaller but more frequent displacement "pop-in" events are observed with increasing load. A change in deformation mode from discrete displacement pop-ins to more continuous "wavy" deformation in specimens < 300 nm in diameter is observed at low strains. Isolated shear bands are visible via high resolution SEM of specimens where testing was interrupted after the first pop-in. However the total shear offset is insufficient to account for the total plastic strain, suggesting that the wavy deformation includes homogeneous flow. Experimental results will be compared with observations of defect evolution from molecular dynamics simulations.

11:10 AM
Effects of Ion-Implantation on Surface Properties and Bioactivity of a Nickel-Free Zr-Based Bulk Metallic Glass: *Lu Huang*[1]; Wei He[1]; Claudiu Muntele[2]; Yoshihiko Yokoyama[3]; Harry Meyer[4]; Daryush Ila[2]; Akihisa Inoue[3]; Tao Zhang[5]; Peter Liaw[1]; [1]University of Tennessee, Knoxville; [2]Alabama A&M University; [3]Tohoku University; [4]Oak Ridge National Laboratory; [5]Beijing University of Aeronautics and Astronautics

The purpose of this study was to investigate the ion-implantation effects on the surface properties and the bioactivity of a nickel-free Zr-based bulk metallic glass (BMG). Polished alloy disks were implanted with Ca and Ar ions, respectively. The stopping and range of ion in matter (SRIM) package was used to simulate the distribution of implanted ions. Surface properties and bioactivity on both treated and untreated samples were characterized and compared. Surface morphology and roughness were examined through atomic force microscopy (AFM). Chemical compositions and depth profiles of the surface layers were obtained using x-ray photoelectron spectroscopy (XPS). The wettability of all substrates was determined by the sessile-drop contact angle method. Corrosion resistance for the untreated alloy was studied in a physiologically-relevant environment. Effects of implantation treatments on cell morphology and proliferation behaviors of bone-forming mouse MC3T3-E1osteoblastic cells seeded on the Zr-based BMGs were investigated.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.

Cast Shop for Aluminum Production: Melt Oxidation, Inclusions and Hydrogen

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

Thursday AM Room: 609
February 18, 2010 Location: Washington State Convention Center

Session Chair: Richard Chandler, Altek-MDY

8:30 AM
Formation of the Solid Layer on the Top of Molten Aluminum: Lucas Nana Wiredu Damoah[1]; *Lifeng Zhang*[2]; [1]University of Ghana; [2]Missouri University of Science and Technology

The formation of the top solid layer on the molten aluminum in launders during refining and casting, constituting production loss, were experimentally, thermodynamically and kinetically investigated in the current study. The effects of humidity and composition of the metal on the oxide layer were discussed. The thickness of the top thin oxide layer was only 1 - 5 µm, and the rest of the top layer averaging 350µm were mainly composed of aluminum matrix with MgO clusters, other inclusions and Fe-rich precipitated phases. Two most feasible reactions out of six were determined to be responsible for the formation of the thin oxide layer. The formation mechanism of the whole top layer was proposed. Higher humidity enhanced the oxidation of molten aluminum while lower humidity favored dissolve [Mg] oxidation. Increasing the humidity reduced the thickness of the oxide formed, however, such increases resulted in increased hydrogen content in the molten metal.

8:55 AM
Removal of Solid Inclusions from Molten Aluminium through Ceramic Foam Filtration: *Alma Engelbrecht*[1]; [1]Hycast AS

A CFF (ceramic foam filter) is commonly found in aluminium cast houses as a final inline melt treatment step before casting. An analytical model to predict the inclusion removal efficiency of a ceramic foam filter has been derived and verified against practical measurements. The model is based on an analogy to the removal of solid particles from a liquid by means of flotation and consists of a simple exponential function of particle size, filter pore size and filtration depth. However, the effects of the melt flow velocity, total inclusion load and the inclusion particle size amongst that of other factors on the operational performance of the CFF have also been studied. It was found that the behaviour of a CFF becomes unpredictable with respect to any model currently available from the literature for certain conditions. This is especially observed for high flow rates and coarse filters.

9:20 AM
Strategies to Reduce Inclusion Input during Liquid Metal Transportation and Melt Distribution while DC Casting of Al Alloys: *Bernd Prillhofer*[1]; Holm Böttcher[1]; Helmut Antrekowitsch[2]; [1]AMAG Casting GmbH; [2]University of Leoben

For the production of high quality rolling ingots, the quality of aluminum melts must be improved along the whole process chain. Furthermore it is absolutely necessary to avoid impurity re-entry after the last melt refinement step in the launder. The inclusion re-entry can be related to oxides, which are generated by surface turbulences in the launder and the melt distribution system of the mould. The most critical phase is the start-up of the DC casting process, which leads to excessive oxide contamination. Finally, the melt distribution bag in the mould has a significant impact on the resulting ingot quality. This paper deals with a reliable methodology to investigate the inclusion input during casting with ultra sonic testing, PreFil® and metallographic analysis, as well as strategies to reduce inclusion re-entry by improved melt flow in the launder. The paper also includes the presentation of special designs of melt distribution systems.

9:45 AM Break

10:05 AM
A New Multi Stage System of Filtration Employing a Cyclone: *John Courtenay*[1]; Frank Reusch[2]; [1]MQP Limited; [2]Drache Umwelttechnik GmbH

The development of a new prototype multi stage filter was described at TMS 2009 in which a ceramic foam filter was applied in a first chamber operating in cake mode; grain refiner added in a second chamber and a cyclone deployed in a final chamber to ensure removal of any oxides or agglomerates arising from the grain refiner addition or release events from the foam filter. The first industrial prototype was installed at Trimet Aluminium at Essen in Germany and demonstrated that liquid metal could pass through the cyclone successfully without excessive turbulence or splash. The further development of the prototype based on new water modeling work together with plant trials is described.

10:30 AM
Hazards Associated with the Use of Bone Ash in Contact with Molten Aluminum: *Don Doutre*[1]; [1]Novelis Global Technology Centre

Bone ash (calcium hydroxyapatite or simply calcium phosphate) has traditionally been used in the cast house to fill cracks, patch holes and cover "make and break" or moveable joints. It has many attractive attributes including its ease of use, low cost and non-wetting characteristics. Bone ash itself is non-toxic and environmentally benign. However recent evidence indicates that bone ash can be reduced upon contact with aluminum alloys to produce metal phosphides. Metal phosphides can in turn react with water or water vapor to liberate phosphine (PH3) a highly dangerous and toxic gas. This paper reviews the observations and experiments that lead to this conclusion and discusses Novelis' search to identify a satisfactory substitute.

10:55 AM
In-Situ Measurement of Dissolved Hydrogen during Low Pressure Die Casting of Aluminium: *Matthew Hills*[1]; Mark Henson[1]; Chris Thompson[1]; Barnett Geddes[2]; Carsten Schwandt[3]; R Kumar[3]; Derek Fray[3]; [1]EMC Limited; [2]Foseco; [3]University of Cambridge

Hydrogen based microporosity is the primary source of defects in Low Pressure Die Cast (LPDC) aluminium wheels, and is one of the most difficult to control. The in-situ measurement of dissolved hydrogen in an LPDC holding furnace is challenging and cannot be achieved by conventional methods such as reduced pressure or circulating gas techniques. A new version of the ALSPEK H probe for the electrochemical measurement of hydrogen in molten aluminium has been developed, and is suitable for deployment in sealed environments. This article presents results of testing under LPDC conditions at a commercial foundry. The probe showed good measurement stability, even during the LPDC pressurised cycle, and responded well to changes in the hydrogen level.

11:20 AM
Hycast SIR- A Unique Concept for Inline Melt Refining: *Idar Steen*[1]; Erling Myrbostad[1]; Terje Haugen[1]; Arild Håkonsen[1]; [1]Hycast

Hycast AS, a Hydro Aluminium subsidiary, developed in the beginning of this decade a new generation of inline melt refining units (I-60 SIR) for the aluminium industry. A traditional gas fluxing principle combined with a unique design, eliminates disadvantages of the conventional degassing systems available today. The I-60 SIR has shown a remarkable high and stable removal efficiency of hydrogen and inclusions from the molten aluminium. The operational costs are low due to very low process gas (Argon) consumption, a drain free reactor and only 2 rotors in operation for a capacity of more than 65 metric tons per hour. The system is a fully automated either as a stand-alone system or integrated in a superior automation system. Installation and verification in more then 90% of the actual Hydro cast houses has been fulfilled, and the concept is now available for the international market.

Characterization of Minerals, Metals and Materials: Characterization of Micro-, Nano-, and Thin Films

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

Thursday AM February 18, 2010 — Room: 306 — Location: Washington State Convention Center

Session Chairs: Ann Hagni, Ann Hagni Consulting, LLC; Toru Okabe, The University of Tokyo

8:30 AM Introductory Comments

8:35 AM

4-D Microstructural Characterization of Snow and Ice: *I. Baker*[1]; R. Obbard[1]; S. Chen[1]; R. Lomonaco[1]; K. Aho[1]; G. Troderman[1]; T. Cassano[1]; [1]Dartmouth College

In this presentation we outline the use of modern analytical techniques to characterize the complete 3-D microstructures of ice and snow firn (multi-year snow) as a function of time. Snow metamorphosis was studied by periodically examining fresh snow over a period of one month, while firn from Summit, Greenland was examined every meter from the surface to pore close off at 90 m, i.e. over several hundred years of snow deposition. The characterization utilized a combination of micro X-ray computed tomography from a unit situated in a cold room and cold-stage scanning electron microscopy, including energy dispersive spectroscopy and electron backscattered patterns.This research was supported by the U.S. National Science Foundation Grants OPP-0738975 and OPP-0821056, and U.S. Army Research Office Contact 51065-EV.

9:00 AM

Characterization of Elastic and Mechanical Properties of Materials by Atomic Force Acoustic Microscopy: *Arnaud Caron*[1]; Shanker Ram[2]; Siddhartha Das[3]; Hans-Jörg Fecht[3]; [1]Institute of Micro- and Nanomaterials, University Ulm; [2]Materials Science Center, Indian Institute of Technology, Kharagpur; [3]Department of Metallurgical and Materials Engineering, Indian Institute of Technology, Kharagpur

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 depend on the contact stiffness k* and thus on the elastic properties of the sample. AFAM can be used as an imaging technique to image the microstructure from the local elasticity cahnges. Also quantitative investigation of the elastic properties of the single phases constituting the microstructure can be carried out. A new application scope lays in the investigation of the contact damping. Here we show how the contact damping may be related to plasticity invents and friction.

9:25 AM

Nanoindentation Analysis as a Two-Dimensional Tool for Mapping the Mechanical Properties of Complex Microstructures: *Nicholas Randall*[1]; [1]CSM Instruments

Instrumented indentation (referred to as nanoindentation at low loads and lowdepths) has now become established for the single point characterization of hardness and elastic modulus of both bulk and coated materials. This makes it a very good technique for measuring mechanical properties of homogeneous materials. However, many composite materials comprise material phases that cannot be examined in bulk form ex-situ (e.g., carbides in a ferrous matrix, calcium silicate hydrates in cements, etc.). The requirement for in-situ analysis and characterization of chemically complex phases obviates conventional mechanical testing of large specimens representative of these material components. This paper will focus on new developments in the way that nanoindentation can be used as a two-dimensional mapping tool for examining the properties of constituent phases independently of each other. This approach relies on large arrays of nanoindentations (known as grid indentation) and statistical analysis of the resulting data.

9:50 AM

Characterization of Nanocrystalline CdS:In Thin Films Prepared by the Spray-Pyrolysis Technique: *Shadia Ikhmayies*[1]; Riyad Ahmad-Bitar[1]; [1]University of Jordan

Nanocrystalline CdS:In thin films with particle size in the range (3-36 nm) were produced by the spray pyrolysis technique on glass substrates. The films were characterized by investigating their X-ray diffractograms (XRD), scanning electron microscope images (SEM), transmittance curves and photoluminescence (PL) spectra. The size of the nanocrystallites was estimated from XRD difractograms and then from the hyperbolic band model and the bandgap energies of the nano-particles, which were calculated from the positions of the minima in the first derivative curve of the absorbance. Fine-structured PL spectra confirmed the nanocrystalline nature of the films.

10:15 AM

Characterization of Nanoscale γ' Precipitates in Ni-Base Superalloys: *Gopal Viswanathan*[1]; R. Srinivasan[1]; J. Tiley[2]; Soumya Nag[3]; R. Banerjee[3]; Hamish Fraser[1]; [1]The Ohio State University; [2]Air Force Research Laboratory; [3]University of North Texas

Nanoscale primary and secondary precipitates from Rene88 DT, a Ni-base superalloy were characterized for their size, morphology, lattice parameters and chemistry as function of selected cooling rates and aging times both in constrained and unconstrained conditions through advanced analytical techniques that include energy- filtered transmission electron microscopy (EFTEM), synchrotron XRD and 3D atom probe tomography (3DAP). The results will be presented and discussed in detail with particular reference to the coarsening kinetics of γ' precipitates with aging time.

10:40 AM

Chemical Co-Deposited PbS – CuS Thin Film Characterization: Effect of Annealing: Mishark Nnabuchi[1]; *Chinedu Ekuma*[2]; Israel Owate[2]; [1]Ebonyi State University; [2]University of Port Harcourt

A heterojunction of PbS – CuS thin film has been grown on glass slides by SGT. The films were annealed for 1hr at temperature of 373K and 423K respectively. The optical properties were characterized using a UNICO UV – 2102 PC Spectrophotometer at normal incidence of light in the wavelength range of 200 – 1000nm. The minimum percentage transmittance was observed to be 34% for sample A and 25% for sample B within the same optical region. The band gap energy was determined from the spectra to be 2.05eV for sample A and 1.85eV for sample B which gave a band shift of 0.20eV. It can thus be concluded that the optical properties of the films within the VIS – UV – NIR can find application in solar thermal technology, particularly as antireflection coating, window materials and as good materials for selective solar cell fabrication.

11:05 AM

Nanosecond Electrical Discharges between Semiconducting Sulfide Mineral Particles in Water: *Igor Bunin*[1]; Valentine Chanturiya[1]; [1]Research Institute of Comprehensive Exploitation of Mineral Resources RAS

Application of high-voltage nanosecond pulses (HPEMP) to disperse mineral media containing particles (from 10 microns to 1 mm in size) of natural semiconducting sulfide minerals leads to electric field concentration at contacts or gaps between neighboring particles due to transient currents through the particles. As a result, conditions for developing electrical discharges between mineral particles are formed. When powder samples, previously moistened or placed in water, are subjected to electric-pulse treatment, particle–particle discharges occur in water; the nature of these discharges differs from that for air gaps. A model for developing electric discharges between sulfide mineral (pyrite) particles under HPEMP-irradiation in a water medium is considered. The probability of electrical breakdowns of liquid gaps between particles depend strongly on the sulfide conductivity. To disintegrate particles with high conductivity, one has to use shorter pulses with a larger voltage amplitude and shorter leading edge, while low-conductivity particles require longer pulses.

11:30 AM
Quantitative Measurement of Volumes for Nanoparticles by High-Angle Annular Dark-Field Scanning Transmission Electron Microscopy: *Helge Heinrich*[1]; Biao Yuan[1]; [1]University of Central Florida

A quantitative method to determine sample thicknesses in Transmission Electron Microscopy (TEM) using the Scanning (STEM) mode is introduced. A High-Angle Annular Dark-Field (HAADF) detector collects electrons scattered to high angles. The intensity of the HAADF signal is proportional to the sample thickness and increases with the atomic number. Multilayered samples provided by TriQuint in Apopka (FL) are used for calibration yielding data on the interaction cross section per atom. With Convergent-Beam Electron Diffraction the thickness of these multilayer systems was measured. Multislice simulations in C# .NET 3.5 are used for comparison with experimental results. These calibrations were applied to determine concentration gradients in nanoscale Fe-Pt multilayers as well as thicknesses and volumes of individual Au-Fe, Pt, Au, and Ag nanoparticles. With this method volumes of nanoparticles with known composition can be determined with an accuracy better than 15%.

11:55 AM Concluding Comments

12:00 PM Question and Answer Period

Characterization of Minerals, Metals and Materials: Characterization of Refractories, Clays, Concrete, Interfaces, and Thermodynamics

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

Thursday AM — Room: 307
February 18, 2010 — Location: Washington State Convention Center

Session Chairs: Jiann-Yang Hwang, Michigan Technological University; Takashi Nagai, The University of Tokyo

8:30 AM Introductory Comments

8:35 AM
Effect of Cold Working on the Thermal Expansion and Mechanical Properties of Fe-29%Ni-17%Co Low Thermal Expansion Alloy: Song-Yi Kim[1]; Jung Namgung[2]; Mun-Chul Kim[2]; *Kee-Ahn Lee*[3]; [1]Center for Advanced Green Materials Technology, Andong National University; [2]RIST; [3]Department of Advanced Material Science and Engineering, Andong National University

The change of thermal expansion and mechanical behavior by cold working and annealing has been investigated in Fe-29%Ni-17%Co low thermal expansion Kovar alloy. Thermal expansion was measured from 25° to 600° with a heating rate of 5°/min by using vacuum differential dilatometer. It was found that thermal expansion coefficient ($a_{30\sim400°X}$) slightly decreased and then remarkably increased with increasing reduction ration of cold rolling. Thermal expansion coefficient sharply decreased after annealing heat-treatment. Yield and tensile strengths continuously increased and elongation decreased by cold rolling. Microstructural observation and X-ray diffraction analysis results showed that the a phase significantly increased as the reduction ratio increased. The slight decrease of thermal expansion coefficient in the early stage of low reduction ratio could be explained by the destroying short-range ordering and the decreasing of grain size. The correlation between the microstructural cause and invar effect of the low thermal expansion behavior was also discussed.

8:55 AM
Thermodynamic Measurement of Phosphorus Oxide in Oxide Systems by Double Knudsen Cell Mass Spectrometry: *Takashi Nagai*[1]; Masafumi Maeda[1]; [1]The University of Tokyo

Thermodynamic information on alloys and oxides forms a scientific foundation for the development of new technologies for refining steel and alloys. Double Knudsen cell mass spectrometry was used as a new method to investigate thermodynamic properties on metals and alloys. In this method, more accurate properties can be estimated easily than those by traditional methods, such as chemical equilibrium method, since pressure of gaseous species in equilibrium with specimens can be measured directly.In this study, this method was applied to measure the properties of oxide systems. The thermodynamic properties of calcium phosphates and other phosphates were estimated by measuring the pressures of gaseous phosphorus and phosphorus oxide in equilibrium with specimen by this method. A new de-phosphorization process in iron and steel industry with multi-phase flux can be proposed with these data, and use of harmful elements for environment and waste slag can be reduced in the process.

9:15 AM
Characterization of Refractories in Gasification Systems Using Post Mortem Analysis and Thermodynamics: *Kyei-Sing Kwong*[1]; James Bennett[1]; Rick Krabbe[1]; Hugh Thomas[1]; [1]NETL

Gasification is a process that converts a carbon feedstock into synthesis gas (CO+H2). Slagging gasifiers operate at high temperature and pressure and in a corrosive-wear environment from the slag. Cr2O3-based refractory linings are used to protect the steel vessel that comprises the gasifier from the aggressive gasification environment. Increasing service life of the gasifier is one of the keys for wide spread development of this technology. In support of the goals, research on the gasifier atmosphere, the slag chemistry, the interaction of Cr2O3 refractory with different feedstock mixtures (e.g., coal and petcoke) were characterized by post mortem analysis of bricks from service in gasifiers and thermodynamics simulation of the environment. Examples demonstrating how thermodynamic calculations can explain the post mortem results and make predictions of material interactions will be given. Attention is placed on the possibility of Cr+6 in different feedstock mixtures and operating conditions

9:35 AM
The Reception of Ceramic Aluminum Silicate Refractories: *Sereda Borys*[1]; Irina Krugljak[1]; Alexandr Zherebtsov[1]; [1]ZSEA

The properties, characteristics and phase structure of chamotte refractories produced with the usage of mullitecorund chamotte and caoline have been given. The comparison of new refractory C-45 obtained by us and refractory C-43 produced by traditional method has done. The physical-chemical properties of refractories is reviewed. The visual porosity, density and pore characteristics of given refractories was calculated. It is established that C-45 has the less gas permeability then C-45 that gives melting units more stability. The petrographical microstructures of refractories have been done. The main phase structures and their influence on refractories properties have been observed. It is established that refractories with mullitecorund chamotte adition has more advantages then refractories gained by traditional method and can be applied to melting units.

9:55 AM
Utilization of Aluminum Slag for the Expansion of Lightweight Concrete: Xuan Li[1]; *Jiann-Yang Hwang*[2]; Hee-Joon Jeon[2]; Matthew Andriese[2]; Zheng Zhang[2]; [1]University of Science and Technology Beijing; [2]Michigan Technological University

Aluminum slag is generated when aluminum metals are recycled through a smelting process in the presence of salt. There are small amounts of aluminum metals trapped in the aluminum slag. This research aims at evaluating the use of aluminum slag as an expansion agent for the production of lightweight concrete by taking advantages of the residual aluminum metals in the slag. The research identified key elements of producing lightweight concrete products through utilizing various mixture components including NaOH, CaO, cement, and gypsum. The volumetric expansion rate was investigated and the density and strength of the products were determined. The results show that aluminum slag can be utilized for the production of lightweight concrete products.

10:15 AM
Characterization of Vitrified Tile Bodies with Kaolinitic Clay and Nepheline-Syenite: *Carlos Maurício Vieira*[1]; Sergio Monteiro[1]; [1]State University of the North Fluminense

This work had for objective to characterize ceramic bodies for vitrified tiles elaborated with the mixture of nepheline-syenite flux and kaolinitic clay. Compositions were prepared with addition of 0, 30 and 50 wt.% of nepheline-syenite to a kaolinitic clay. The firing behavior of the compositions was evaluated by optical dilatometry. Specimens were prepared by uniaxial pressure at 30 MPa followed by firing at 1175°C. The fired specimens were submitted to the following tests: bulk density, linear shrinkage, three point bending mechanical strength and water absorption. Microstructural analysis was carried out by scanning electron microscopy. The results showed that the formulations with nepheline-syenite have a potential to obtain vitrified ceramic, by significantly decreasing the porosity of the pure clayey ceramic.

10:35 AM

Systematic Study of Bentonitic Clay and Quaternary Ammonium Salts: Renata Barbosa[1]; Dayanne Souza[1]; Karine Nóbrega[1]; *Edcleide Araújo*[1]; Tomás Mélo[1]; [1]UFCG

Besides the vantage of the abundance of bentonitics clays in the Brazil and the modification of these clays by surface treatment with quaternary ammonium salts is a simple method. In this work, it was made a previous study with four different ammonium salts and a bentonitic clay. The clay was characterized by cationic exchange capacity, determinantion content of montmonrillonite, X-ray fluorescence and X-ray diffraction. The salts were characterized by Differential Scanning Calorimetry and Thermogravimetry. Then, a salt with thermal stability was selected for organophilization. It was observed that some ammonium salts are more thermally stable than others and with near values of decomposition temperature. The results of DSC and TG indicated that the salts with chloride anion (Cl-) decompose first and the salt with bromide anion has more thermal stability. The evidence of the incorporation of the quaternary ammonium salts in the clays structure was seen by XRF and XRD.

10:55 AM

Technological Characterization of Serpentinite Rock from Andorinha (Bahia/Brazil): *Aline Maria Teixeira*[1]; João Sampaio[2]; Francisco Garrido[3]; Marta Medeiros[3]; [1]IQ/UFRJ - CETEM; [2]CETEM; [3]IQ/UFRJ

Serpentinite is an ultra basic and metamorphic rock consisting mainly of magnesium, calcium and silicon oxides. The rock under study is a host rock of chromite mine located in Andorinha, BA. The objective of this paper is to evaluate the rock's physical and chemical characteristics to be used as an additional fertilizer of acid soils. After comminution, rock samples were submitted to chemical analysis, XRD, SEM-EDS and TGA. Afterwards, particle size distribution was determined. Result analysis confirms that our rock consists mainly of dolomite, calcite and diopside. According to the result obtained, it can be said that the serpentinite rock has promising applications in agriculture for the correction and additional fertilization of acid soils. However, it is necessary to study the characteristics of the rock such as its dangers and toxicity as well as evaluate them according to the legislation for corrective acidity.

11:15 AM

Properties and Durability of Ready Mix Repair Mortars in Hot Environment: *Benchaa Benabed*[1]; [1]University of Laghouat

The main objective of this work is to study the physical and mechanical properties and durability of ready mix repair mortars. The experimental study was carried out on four types of repair mortars (one hydraulic mortar, a micro-concrete a mortar with latex and a mortar containing fibers and silica fume). The properties of the repair mortars at the fresh and hardened states are analyzed. The effect of humid curing using Hessian regularly humidified, on the mechanical properties in hot and dry environment was also studied. The results of the experimental study showed that the repair mortar containing silica fume gave a better compressive strength in all curing environments. The study showed also the negative effect of hot and dry environment on all types of ready mix repair mortars and demonstrated the importance of humid curing during early age.

11:35 AM Concluding Comments

11:40 AM Question and Answer Period

Electrode Technology for Aluminum Production: Preheating and Operational Aspects

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

Thursday AM — Room: 616
February 18, 2010 — Location: Washington State Convention Center

Session Chair: Paulo Douglas Vasconcelos, Albras Alumínio Brasileiro S.A

8:30 AM Introductory Comments

8:35 AM

Loss in Cathode Life Resulting from the Shutdown and Restart of Potlines at Aluminum Smelters: *Alton Tabereaux*[1]; [1]Consultant

The loss in potlife that results from the shutdown of aluminum cells in potlines is primarily due to cathode cooling that occurs in potlines when the amperage is significantly reduced or when the power is interrupted. Cooling cells from 955°C to ambient, 25°C, results in irreversible and non-repairable damage to the cathodes. Cooling ultimately result in the formation of numerous long 'cooling' cracks on the surface of cathode blocks and in the seams between blocks. The impact of uncontrolled vs. controlled shutdown of cells in potlines is discussed. The amount of loss in potlife can be substantially different for potlines at smelters depending upon the circumstance of the cathodes at the time of the potline shutdown as well as the potline restart method.

8:55 AM

Investigation of the Impact of Pre-Heating, Start-Up and Early Operation on Potlife: *Jayson Tessier*[1]; Carl Duchesne[1]; Gary Tarcy[2]; Claude Gauthier[2]; Gilles Dufour[2]; [1]Laval University; [2]Alcoa Inc

Industrially, aluminium is produced inside metallurgical reactors, known as reduction cells or pots. Given that a few hundreds to a thousand of cells are operated in a smelter and because these pots have a typical life span of 4 to 10 years, replacing and starting pots is almost a common operation in a smelter. Once in place, new cells are pre-heated, started and operated. It is believed that pots experiencing upsets during these steps may give a lower potlife. This study presents a statistical analysis based on 31 started pots from the Alcoa Deschambault smelter. Using different statistical tools, it is demonstrated that enough information is enclosed in the pre-heating, start-up and early operation steps to perform a meaningful potlife prediction, on a pot-to-pot basis, a few weeks after start-up. Prediction results are discussed and the model structure is investigated to find variables having the greatest influence on potlife.

9:15 AM

Evaluation of Mothballing and Subsequent Restarting of Søderberg Cells: *V.Yu. Buzunov*[1]; V. I. Borisov[1]; Ye.G. Masyutin[1]; D.G. Bolshakov[1]; A.A. Pinayev[1]; [1]RUS-Engineering Ltd.

In view of the latest economic changes, the world aluminium producers have stopped the least cost-effective production capacities, reducing process costs and aluminium supply to the market trying to keep the price at an acceptable level. For choosing a mothballing technology some basic requirements were taken into consideration: - minimum costs on cells shutdown, heating and restart; - minimum influence on the cell's death age. In this paper we present our evaluation of two mothballing methods: the partial and complete metal tapping out from the cathode for vertical stud Søderberg cells.

9:35 AM

Analysis of the Coke Bed Preheating Method for Aluminium Cells: *Mohamed Ali*[1]; [1]The Aluminium Company of Egypt

Resistor coke bed preheating method is the most common method used in aluminium cells preheating. This was based on typical start-up anode effect as well as typical cathode heat-up rate during preheat and start-up. The drawbacks of this method were studied and modified to give the best performance for cells preheating. These modifications include coke bed thickness, preheating time, using flexible anode connections, fixing cathode carbon blocks and ramming paste sources and adaptation the procedures for preheating. These modifications improved from pot lives, and lowered the electrical energy and coke consumption during the preheating process. Also, the effect of workers experience on the performance of preheating was studied.

9:55 AM
The Combined Flame and Aluminum Preheating Method: Tian Yingfu[1]; *Feng Naixiang*[2]; Peng Jianping[2]; Wang Yaoyu[2]; Li Jian[3]; [1]Chongqing Tiantai Aluminum Industry Co., Ltd.; [2]Northeastern University; [3]Jianwenyuan Industrial Equipment Company

A combined Flame-Aluminum-Preheating (FAP) method for aluminum electrolysis cells is presented. This preheating process includes two steps. In the first step the aluminum electrolysis cell is preheated to 700~800° by the flame from gas burning, and in the second step about 8 tons of liquid aluminium are poured into the cell, and the cell is then preheated to 950° by electrical heating. The FAP method has been applied successfully in three 168 kA novel cathode cells at the Tiantai aluminum smelter in China. This shows that the FAP method is simple, safe and reliable, and it gives a short preheating time and low energy consumption of 12400 kW•h and gas consumption of 2500 m^3.

10:15 AM Break

10:30 AM
Cell Preheat on Full Line Current at Dubal: *Ali Al Zarouni*[1]; Maryam Al Jallaf[1]; Arvind Kumar[1]; K. Alaswad[1]; J. Blasques[1]; [1]DUBAL

Main objective of cathode preheating is to achieve an optimum cathode life by pyrolyzing the bonding pitch and gradually raising the temperature of the lining material close to the normal operating temperature of the cell. The risk of thermal stresses and melt penetration can be minimised by adopting a good preheat and start up procedure. Resistive preheating on full line current was tried out by initially using a mixture of CP coke and graphite and later by using 100% graphite as heat transfer and resistance media. By doing so, resistor material consumption dropped by 93%, preheat energy was reduced by 10%, use of compressed air to cool shunts was eliminated and hardly any skimmings following bath up. The method permits accelerated start up especially in expansion projects and in restarting a potline following power outage. A techno-economic evaluation shows the method contributes to higher productivity at lower cost.

10:50 AM
Optimization of the Anode-Stub Contact: Material Properties of Cast Iron: *Bjarte Oye*[1]; Elin Haugland[2]; Jorund Hop[2]; Arne Nordmark[1]; Morten Onsoien[1]; [1]SINTEF; [2]Hydro Aluminium

Contact between the anode and the anode stub is normally made by cast iron. Important parameters are the iron fluidity during casting and the subsequent dimensional changes during cooling and the first heat-up. Three qualities of cast iron were investigated; standard grey iron with and without inoculation, and non-inoculated iron with 0.5 percent added phosphorus. The main contributor to fluidity appeared to be the temperature, as the metal flow when cast from 1350 °C was twice the length found at 1250 °C. Only minor differences were observed between the iron qualities, where the ordinary grey iron performed best. The cooling shrinkage of inoculated iron was lower than for the non-inoculated, probably because of an advantageous graphite structure obtained during the ferrite transition. Only minor differences were observed for the non-inoculated alloys. During the first heating, high phosphorus irons expanded significantly more than the rest at temperatures above 600°C.

11:10 AM
Voltage Drop, Stub-Anode Connection, Cast Iron: *Adel Nofal Adel Nofal*[1]; Mohamed Waly[1]; Ahmed Ahmed[1]; Mahmoud Agour[1]; Amr Kandil[1]; Shaher Mohamed[1]; Mohamed Mourad[1]; [1]Aluminium Company of Egypt

This paper studies the influence of the carbon equivalent (CE) of grey iron on the electrical resistance of the stub-anode connection. Three levels of CE were studies i.e. 3.9, 4.3 and 4.5 through changing the Si-content, the effect of increased P-content was also studied.A bench-scale experimental set-up was used to simulate the operating conditions at the steel stub / cast iron collar / carbon anode. The change in microstructure and electrical resistance was measured at temperatures up to 850°C. up to 30 days. The thermal expansion properties of different cast iron grades and of the steel stub were measured using a high precision automatic dilatometer. The electrical resistance at the stub / collar / anode connection was related to both the electrical resistivity of the iron collar and the contact pressure, which was found to depend on the cast iron graphitization favoured by high CE-values.

General Abstracts: Electronic, Magnetic and Photonic Materials Division: Session II

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

Thursday AM — Room: 308
February 18, 2010 — Location: Washington State Convention Center

Session Chair: To Be Announced

8:30 AM Introductory Comments

8:35 AM
Chemical Vapor Transport Synthesis and Optical Property of Moo_3 Thin Film: Young Jung Lee[1]; Chang Won Park[1]; Dae-Gun Kim[1]; *Young Do Kim*[1]; [1]Hanyang University

Transition metal oxides have attention in the industrial application fields of photochromic, electrochromic, sensor, catalyst and electrode for microbatteries. Among them, MoO_3 thin films have been extensively investigated in the electrochromic (EC) device field due to its superior optical properties. Recently, many deposition techniques to deposit Mo oxide thin films have been developed. In this study, new deposition technique for the successful deposition of homogeneous MoO_3 thin films was accomplished through the chemical vapor transport of volatile $MoO_3(OH)_2$ during the reduction of MoO_3 powder and subsequent thermal annealing. As annealing commenced, the optical transmittance of the films increased due to enhancement of the crystallinity resulted from oxygen vacancy reduction and increase of the relative density from reduction of porosity. Also, electrochromic property of the annealed MoO_3 thin film was analyzed by intercalation of ions in $LiClO_4$ dissolved in propylene carbonate (PC) as electrolyte.

8:55 AM
Improved Performance of a Fluorescent Blue Organic Light Emitting Diode with Hole Blocking Materials as Dopants for Transport Layers: Girija Samal[1]; K. N. Narayanan Unni[1]; Saswat Bharat[1]; *Deepak*[2]; [1]Samtel Color Ltd; [2]Indian Institute of Technology Kanpur

Realizing a highly efficient deep blue organic light emitting diode (OLED) with sufficient life time is the biggest challenge in the fabrication of full color OLED displays. Using hole blocking layers (HBL) has been an established technique to confine excitons or carriers in the recombination region. In the present work, we have doped the hole transport layer (HTL) and electron transport layer (ETL) with two different hole blocking materials and compared the performance of these devices with that of a standard device. Our standard blue OLED demonstrates a current efficiency of 2.3 cd/A. To improve its current efficiency, we have doped the ETL by a hole blocking material (BPhen), which shows no improvement in current efficiency. But, doping the HTL with another hole blocking material (TPBi) has led to current efficiency as high as 4.3 cd/A. The importance of band gap engineering is discussed based on the above studies.

9:15 AM
Luminescence of the GaP:N Long-Term Ordered Single Crystals: *Sergei Pyshkin*[1]; John Ballato[2]; Andrea Mura[3]; Marco Marceddu[3]; [1]Academy of Sciences; [2]Clemson University; [3]The University of Cagliari

GaP:N single crystals were prepared by one of the authors (SP) during 1963-1966 using the method of free crystallization from Ga solution. It is known that the characteristic time of the substitution reaction during N diffusion along P sites in GaP:N crystals at room temperature constitutes 15-20 years. Hence, the observations of highly excited luminescence of the crystals made in the sixties and the nineties were then compared with the results obtained in 2009 in closed experimental conditions. The impressive nearly semi-centennial evolution of the GaP:N luminescence observed is interpreted as the result of both volumetrical

N impurity ordering and the formation of an ordered bound exciton system at some level of optical excitation. The highly ordered nature of this new host and excitonic lattices increases the radiative recombination efficiency, and makes possible the creation of advanced non-linear optical media for optoelectronic application.

9:35 AM
Opals, Photonic Band Gap Materials, Pleochroic Refraction, and Monochromatic Lasers: *Michelle Stem*[1]; [1]University of Texas at El Paso

Opals embody the application of Bragg's Law over visible light. Here, fundamental research was applied to natural opals because they are used to develop photonic band gap (PBG) material templates. Effects from applying two laser wavelengths (532nm and 630-650nm) and tungsten white (580-590nm) to the many types of natural opal were compared. The ranges of many traits of opals includes: opaque to transparent, vibrant to colorless, diffuse to refraction. Because some types of opals (transparent and refraction) exhibit at least partial PBG control, a comparison of refraction and colors refracted relative to incident angles were determined for each photon source. This research determined whether only polychromatic light caused certain opals to refract different wavelengths in different directions or if the monochromatic lasers caused the same opals to have different refraction wavelengths or different directions. Opal-based materials are transforming the computer industry, especially for NOEMS and MOEMS materials.

9:55 AM Break

10:15 AM
Coercivity Enhancement of Nd-Fe-B Sintered Magnets by Two-Step Sintering: Se Hoon Kim[1]; Hoon-sup Kim[1]; Jin Woo Kim[1]; Dae-Gun Kim[1]; *Young Do Kim*[1]; [1]Hanyang University

Nd-Fe-B sintered magnets are normally composed of $Nd_2Fe_{14}B$ hard magnet phase as matrix and Nd-rich phase on grain boundary. Many researchers have shown that the coercivity of Nd-Fe-B magnets was sensitive to microstructure, such as the grain boundary phases and grain size, etc. Therefore, modifying a sintering process has been an important method for better homogeneous microstructure. In this study, Nd-Fe-B powder was compacted under magnetic field of 20kOe. After that, the green compact was sintered at 950°C for 4h as first-step and second-step sintering was performed as 1050°C. The microstructure was investigated by TEM and EPMA. Magnetic properties were measured by a B-H tracer. Densification over 99% could be obtained by the two-step sintering of Nd-Fe-B powder under 6μm in $Nd_2Fe_{14}B$ phase and the Nd-rich phase was homogeneously distributed around $Nd_2Fe_{14}B$ phases. Moreover, the two-step sintering process led to uniform grain size distribution which had the improved magnetic properties. This research was supported by a grant from the Fundamental R&D Program for Core Technology of Materials funded by the Ministry of Knowledge Economy, Republic of Korea.

10:35 AM
Structure and Magnetic Properties of Fe-Co-Ni-Zr-B-Cu Nanocrystalline Soft Magnetic Alloys: *Keith Knipling*[1]; Maria Daniil[1]; Matthew Willard[1]; [1]Naval Research Laboratory

Nanocrystalline soft magnetic materials possess a unique combination of large magnetization, high permeability, and low core losses. In these materials, nanoscale ferromagnetic grains are exchange-coupled through a surrounding amorphous matrix, minimizing magnetocrystalline anisotropy and improving the magnetic performance. This exchange-coupling is eliminated, however, above the Curie temperature of the intergranular amorphous phase, limiting the maximum service temperature of the alloys. The effect of substituting Co and Ni for Fe in a series of $Fe_{88-2x}Co_xNi_xZr_7B_4Cu_1$ alloys (x = 0–22) are presented. Magnetization generally decreases and the coercivity increases with increasing x, whereas the Curie temperature of the amorphous phase increases significantly (from 73°C at x = 0 to 570°C at x = 22). There is thus an optimum composition near x = 5.5 exhibiting excellent soft magnetic properties at 300–500°C. The performance is competitive with extant Co-based alloys but at much lower costs by virtue of the high Fe content.

General Abstracts: Electronic, Magnetic and Photonic Materials Division: Session III

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

Thursday AM — Room: 310
February 18, 2010 — Location: Washington State Convention Center

Session Chair: To Be Announced

8:30 AM Introductory Comments

8:35 AM
A Subatomic Particle Electromagnetic Wave Solution In A Simplified Space/Time Environment: *John Elton*[1]; James Cornwell[1]; [1]Protective Systems, Inc.

The derivation of the electromagnetic wave functions for subatomic particles using Maxwell's equations is described. This solution demonstrates how Heaviside and Dirac Delta functions can be used to solve Maxwell's equations at a point. Fundamental relationships between electromagnetic variables will be discussed and physical constants of selected subatomic particles will be determined. Using these solutions the rest mass of subatomic particles can be represented and the fundamental relationship between energy, rest mass and momentum can be derived.

8:55 AM
Effect of Electroplating Bath Temperature on Sn Surface Morphology: *Uttara Sahaym*[1]; Stephanie Miller[2]; M Norton[1]; [1]Washington State University; [2]University of Illinois

The present study documents the effect of electroplating bath temperature on the surface brightness/reflectivity and the evolution of surface morphology of electrodeposited pure Sn films, and its subsequent effect on whisker formation. The brightness/reflectivity of the films increased with increase in temperature. Detailed microstructural analysis of the electroplated Sn films showed that unique pyramid shaped features formed at elevated temperatures (below 85°C) and the underlying surface became increasingly smooth with temperature. The plating temperature also affected the morphology of the whiskers that formed upon aging at room temperature. The whisker diameter increased whereas the size decreased with increase in plating temperature. It was also observed that the diameter and length of each whisker depends on the Sn grain size. The growth mechanisms of pure Sn films and the development surface morphology during electrodeposition at different temperatures will be discussed.

9:15 AM
Introduction of Digital Field Control System in Skelp Mill, DSP: *Tapas Kanti Dutta*[1]; Goutam Majumder[2]; Suresh Sarkar[2]; Nilay Gupta[2]; Shaktiveer Singh[1]; [1]RDCIS, SAIL; [2]Durgapur Steel Plant, SAIL

In Skelp mill of Durgapur Steel Plant, the roughing stands consisting of six horizontal stands and three vertical stands (edgers), are driven by DC motors with one common armature voltage. The finishing stands, consisting of five horizontal stands are driven by another common armature voltage. The two armature voltages are generated by two separate thyristor converters. The fields of the motors are controlled to obtain speed regulation. There was no correction of speed drop due to impact of biting and operation of the mill motors over entire speed range could not be achieved. Absence of on-line diagnostics led to increase in downtime in case of mill breakdown. Introduction of this scheme has resulted in faster response (faster speed drop correction), possibility of setting speed over entire speed range, reduction in down time and operator's satisfaction to run the mill.

9:35 AM
The Photophysics of a Luminescent Ruthenium Polypyridyl Complex with Pendant β-Cylodextrin; pH Modulation of Lifetime and Photoinduced Electron Transfer: *Muath Atmeh*[1]; [1]National University of Ireland

We have conducted detailed photophysical studies on the luminescent host [Ru(bpy)2(phen-CD)]2+. The complex exhibits a strong pH dependent luminescence, which is attributed to protonation/deprotonation of the secondary amine bridge linking the CD and ruthenium polypyridyl centre. From emission studies, the pKa for the amine was determined to be 11.5. [Ru(bpy)2(phen-CD)]2+ forms host guest complexes with AQ and AQC, with association constants of 4,920 ± 560 M–1 and 14,657 ± 2,200 M–1. The anthraquinone guest appears to participate in efficient photoinduced electron transfer from the excited ruthenium polypyridyl centre. The possibility that protonation/deprotonation at the amine linker can be used to modulate electronic communication between the CD and luminophore was explored. However, the rate of photoinduced electron transfer appeared to be relatively insensitive to the state of protonation of the bridge.

9:55 AM
Materials and Manufacturing Challenges in Hybrid Flexible Electronics: *Khershed Cooper*[1]; [1]NRL

Flexible electronics is a relatively new field involving electronic or optoelectronic devices on flexible substrates. It is a silicon-based technology necessitating ingenious ways of laying down the brittle silicon and other semiconductors on plastic substrates. Hybrid flexible electronics is an emerging technology of considerable promise. Conformable, foldable, stretchable, rollable and deformable electronic devices are possible. A key ingredient is organics, which opens up the material selection window significantly for the development of semiconductors, dielectrics and other electronic components. However, to advance hybrid flexible electronics, there is a pressing need for research in thin-film organic-inorganic hybrid circuits, devices and systems and high throughput, roll-to-roll manufacturing requiring high resolution and accurate registry. An in-depth understanding of materials behavior and fabrication issues should advance the field greatly so applications such as lighting, photovoltaics, batteries, displays, e-paper, sensors, actuators, RFIDs on flexible substrates can be realized.

10:15 AM Break

10:35 AM
An Experimental Setup and Procedure for Thermal Resistance Measurements of a Thermal Interface Material: *Kaustubh Kalkundri*[1]; Frank Andros[1]; Bahgat Sammakia[1]; [1]SUNY at Binghamton

Increasing functionality while concurrent scaling has put demanding requirements on the reliability of silicon devices due to the resultant increase in power dissipation. A test apparatus was developed for steady state thermal resistance measurements of a Thermal Interface Material (TIM) based on Fourier law. The primary objective to develop a measurement system compatible with industry needs for repeatable measurements was realized by using a commercial thermally conductive epoxy adhesive as TIM. Experiments performed determined interface thermal resistance of assembled test samples as a function of their Bond Line Thickness. An uncertainty analysis was performed to find the maximum potential variation in the thermal resistance and emphasize on the selection of appropriate equipment for measurements. It was verified that increasing the heat flow and BLT reduces the uncertainty in interface temperature difference. Furthermore, modeling was used to understand the impact of defects in the TIM interface.

10:55 AM
Effect of Isothermal Aging and Thermal Cycling on Interfacial IMC Growth and Fracture Behavior of SnAgCu/Cu Joints: *Xiaoyan Li*[1]; [1]Beijing University of Technology

The growth of IMCs of SnAgCu/Cu solder joint in isothermal aging and thermal cycling, was investigated with the focus on the growth kinetics. The joints were isothermal aged at 125C, 150C and 175C while the thermal cycling was performed on -25C to 125C and -40C to 125C. The tensile strength was evaluated by in-situ tensile test. It was found that the grain size of IMCs increases and their morphology were changed. The thickness of IMCs was found increases with the thermal cycles but the growth rate was less than that of thermal aging. The growth of IMCs was found follows Arrhenius's diffusion model and the corresponding diffusion factor and active energy were obtained. The tensile strength of the joints decreases with the increase of aging time while the fracture site was moved. The shear strength was found decrease with the increases of the thermal cycles.

11:15 AM
Magnetic Properties of New Diluted Ferromagnetic Semiconductors $Pb_{1-x-y}Mg_xCr_yTe$: *Elena Zvereva*[1]; Olga Savelieva[1]; Sergey Ibragimov[1]; Evgeny Slyn'ko[2]; Vasily Slyn'ko[2]; [1]Moscow State University; [2]Institute of Material Science Problems

The temperature and magnetic field dependencies of the magnetization (T=1.8-300 K, B ≤ 7 T) and X-band EPR (f=9.1-9.6 GHz, B ≤ 0.7 T, T=80-400 K) has been studied for novel diluted magnetic semiconductors $Pb_{1-x-y}Mg_xCr_yTe$. It was shown that all samples are ferromagnetic with the Curie temperature up to T=275 K. Magnetic saturation is achieved at magnetic fields higher 5 T. With increasing of the chromium content the magnetic saturation moment increases and achieves 0.2 emu/g. The temperature dependencies of the magnetization M(T) is rather concave type with a broaden maximum at temperature about 115 K. EPR spectra in the paramagnetic phase were satisfactory approximated by a single Dysonian line with the typical linewidth about 600 G. In ferromagnetic phase pronounced distortion and splitting of the EPR spectra on two Dysonian lines were revealed. Temperature dependencies of the effective g-factor and the line width for each absorption line were obtained.

11:35 AM
Structure and Properties of Metamagnetic Functional Alloys Ni-Mn-In: *Pnina Ari-Gur*[1]; Michael Morris[1]; Gregory Huizenga[1]; Victor Koledov[2]; Vladimir Shavrov[2]; Vladimir Zolotorev[2]; Alexander Kamantsev[2]; Vladimir Khovailo[2]; Fernando M. Araujo-Moreira[3]; Oscar F. de Lima[4]; [1]Western Michigan University; [2]Kotelnikov' Institute of Redioengineering and Electronics of RAS (Moscow); [3]Universidade Federal de São Carlos (Brazil); [4]Universidade Estadual de Campinas (Brazil)

Metamagnetic Shape Memory Alloys (SMA) Ni-Mn-In demonstrate unique properties of both giant magnetic field-induced strains and giant magnetocaloric effect. This is due to the phenomenon of the thermoelastic martensitic transition, giving rise to shape memory effect, merging with the metamagnetic phase transition from ferro to antiferromagnetic state. In the present work, the samples of metamagnetic SMA Ni-Mn-In were prepared and their structure, magnetic properties and phase transitions studied. The clear thermally-induced shape memory effect has been demonstrated. In situ neutron diffraction tests showed the effect of magnetic-field-induced structure transformation near metamagnetostructural transition temperature.

General Abstracts: Light Metals Division: Session III

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

Thursday AM Room: 607
February 18, 2010 Location: Washington State Convention Center

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

8:30 AM
Multistage Fatigue Modeling for Three Wrought Al Alloys: *Yibin Xue*[1]; [1]Utah State University

Wrought aluminum alloys are primary materials in aerospace and automotive vehicular body structures. Alloying, casting, wrought process, heat-treatment/aging, and final form establish distinct composition, microstructural features, and hardening mechanisms of wrought Al alloys, which also alter fatigue behaviors. Solution treated, age-harden 2xxx, precipitate hardened 6xxx, and solution heat treated, precipitation hardened 7xxx Al alloys, are chosen for multistage fatigue modeling excises. Presumably, all alloys are tempered for the highest achievable strength. The physically motivated mechanistic MultiStage Fatigue (MSF) model are developed for the three alloys based on the static, cyclic, limited fatigue behaviors, and micromechanical simulations. The differences in fatigue damage incubation mechanisms are identified and incorporated into the MSF model according to the accumulated microplasticity associated with the incubation mechanism. The first-order MSF model developing methodology is proposed and the MSF model predicts fairly coherent upper and lower bounds of fatigue lives in the high cycle fatigue regime.

8:50 AM

Optimised Fatigue Behaviour of Ti-6Al-4V Alloy Components Fabricated by MIM: *Orley Ferri*[1]; Thomas Ebel[1]; Rüdiger Bormann[1]; [1]GKSS - Reasearch Centre

During the last few years, processing of Ti-6Al-4V alloy powders by Metal Injection Moulding (MIM) has gained increasing interest in research and applications. Nowadays, it is possible to manufacture MIM Ti-6Al-4V alloy components with tensile properties comparable to those of the wrought material. In contrast, the fatigue behaviour of MIM components does not follow the same trend. In order to improve the fatigue behaviour of MIM components, the critical microstructural features and process parameters were identified. The results showed that grain size is more important than remaining porosity and impurity levels. Based on this result, a beneficial microstructure was obtained by adding amorphous boron powder in the range of 0.1 to 0.5 wt.% to Ti-6Al-4V alloy powder during the MIM process. Excellent tensile (σ_y = 790 MPa, UTS = 900 MPa, ε = 12%) and fatigue (endurance limit ~ 640 MPa) properties were achieved by adding 0.5 wt.% boron.

9:10 AM

Structural Analysis of Hot Blow Formed Aluminum Center Pillar with Residual Stress Consideration: *Dongok Kim*[1]; Jinpyeong Kim[1]; Yongmun RYU[1]; [1]KATECH

Hot blow forming has been introduced to automotive industries since it makes super-plastic forming possible for the materials which has been considered to be difficult to form. Although its low production rate due to the limitation of the allowed strain rate is the disadvantage, by applying this process complex shapes of the metal sheet can be achieved in one piece and the absence of weld and rivet can reduce the risk for fatigue damages. However, many studies have carried out the structural analysis without the consideration of residual stress after hot blow forming. In addition, the material properties of aluminum alloys after hot blow forming have not been applied to the analysis. Therefore, in this study, the structural analysis of hot blow formed center-pillar with considering changed material properties and residual stresses has been carried out to achieve more precise prediction of finite elemental analysis.

9:30 AM

Thermo-Mechanical Characterization of Al-Cu-Mg Composites Reinforced with Diboride Particles: *Natalia Cortes*[1]; Pilar Barrado[1]; Sergio De Hoyos[1]; Hermes Calderón[1]; Oscar Suárez[1]; [1]University of Puerto Rico-Mayaguez

Aluminum-based composites are being evaluated for aerospace and transportation applications where light weight and appropriate strength at high temperatures are key requirements. The present work focused on the mechanical response of a series of Al matrix composites at room and high temperature. The composite matrix contained 2.5 wt.% Cu and 1 wt.% Mg and was reinforced with different levels of boron (0, 1, 2, 3 and 4 wt.%) forming AlB_2 particles. The specimens, fabricated via gravity casting, were tested using a Thermo-Mechanical Analyzer (TMA) under constant compression loads. This TMA instrumentation also permitted studying creep response of the composites. Our results indicated that even at 300ºC higher concentration of diboride particles helped the composite retain high hardness compared to an unreinforced alloy with similar concentrations of Mg and Cu.

9:50 AM

Upgrade and Electrochemical Reduction of TiO2-Rich Slag to Titanium: *Qian Xu*[1]; Ling Sun[1]; Qiu-Shi Song[1]; Wei Xing[1]; Ji-Hong Du[2]; Zheng-Ping Xi[2]; [1]Northeastern University; [2]Northwest Institute for Non-Ferrous Metal Research

An upgraded titania slag with more than 95% mass percent TiO2 was produced by alkali fusion and acid leaching of TiO2-rich slag prepared by electrical furnace smelting. The influence of various experimental conditions on the chemical composition of the upgraded titania slag has been investigated, such as the amount of alkali used, reaction time, HCl concentration for leaching and final pH. The mechanism of the alkali fusion-acid leaching process is studied by X-Ray diffraction and Fourier Transform Infrared spectrometry. The upgraded titania slag was compacted to the thin pellets, then sintered at 900°, and finally electrochemical de-oxidized to titanium.

10:10 AM Break

10:30 AM

Wear Behaviour of the Newly Developed Biomedical Beta Titanium Alloy (Ti-23Nb-0.7Ta-2Zr-1O): *Sathish Sathyavageeswaran*[1]; M. Venkatesh[1]; Geetha Manivasagam[1]; Asokamani Rajamanickam[1]; T.K. Nandy[2]; [1]VIT University; [2]Defence Metallurgical Research Laboratory

Inspite of superior mechanical properties such as low modulus of elasticity, high strength to weight ratio and excellent biocompatibility among the biomedical titanium alloys, it suffers from poor wear resistance. The objective of this work is to enhance the wear resistance of the newly developed beta titanium alloy, gum metal (Ti-23Nb-0.7Ta-2Zr-1O) by subjecting it to various heat treatments. These alloys were subjected to α and β solution treatments and its mechanical properties were measured. Phase analysis was performed using X-ray diffraction technique and microstructural observations were made using scanning electron microscopy. The sliding wear behavior of all these heat treated samples were studied under simulated body fluid (Hank's solution) condition and compared with the conventional Ti-6Al-4V and β-CEZ alloys. The results of the above studies will be discussed in detail in this paper.

10:50 AM

Friction Stir Spot Welding of Magnesium Alloys: *Qi Yang*[1]; Xiang Li[1]; Ke Chen[1]; [1]Hitachi America, Ltd.

Friction stir spot welding, as a derivative of friction stir welding, has been developed for joining body structures. In the present study, AZ31, AM30, and AM60 magnesium alloys are friction stir spot welded with different material combinations and welding configurations. The effect of process condition on macrostructures, microstructures and strengths of spot welds is investigated. Higher weld strength is obtained at a lower rotation speed. Furthermore, spot welds of dissimilar materials could show higher strength than spot welds of the same materials.

11:10 AM

Study on the Materials of Rolled Al-Mg-Si Alloy Used for the High-Speed Trains: *Kai Ji*[1]; Guangchun Yao[1]; Yongliang Mu[1]; Guoyin Zu[1]; [1]School of Materials & Metallurgy, Northeastern University

Based on 6082 aluminum alloys, an novel Al-Mg-Si alloy was designed, which possesses strong weldability and corrosion resistance. Through the orthogonal test, effects of adding slight Mg, Mn, Cu and Cr on strong weldability and corrosion resistance was analyzed.The results show that the best composition design of rolled Al-Mg-Si alloy was Mg 1.0%, Si 0.8%, Mn 0.70%, Cu 0.40%, Cr 0.20%. Moreover, the appropriate technology of TIG welding has been found to improve the mechanical properties of the welds due to grain refinement occurring in the fusion zone. The joint efficiency by ER5356 welding wires reached up to 78%. Finally, silicon and copper were concentrated at the dendrite boundaries and a-Al + Si + Al2Cu + Mg2Si eutectic was observed by optical (OM) and scanning electron (SEM) microscopy. Coarse dimples and voids had been observed in the fractographs. The joints show a transgranular type failure.

11:30 AM

Thermodynamic Design of Ultra-Strong Titanium Alloys Undergoing Plasticity Induced Martensitic Transformations: *Suresh Neelakantan*[1]; Pedro Rivera-Diaz-del-Castillo[2]; Sybrand van der Zwaag[2]; [1]Materials Innovation Institute/Delft University of Technology; [2]Delft University of Technology

Our previous work has shown that the strength of β titanium alloys can be increased up to 50 % via inducing martensitic transformations under plastic deformation, without compromising on other properties such as ductility. Tailoring such transformations for various alloy compositions and deformation temperatures may be performed with the aid of thermodynamic computations. Inspired by Ghosh and Olson's theory for martensite formation in ferrous systems *[Acta. Met., Vol. 42, pp. 3361, 1994]*, a thermodynamic framework is presented to control Plasticity induced transformations in titanium alloys; and its application in developing novel alloys, subjected to various deformation schemes is presented. The prospects of developing a new family of metastable β alloys displaying improved strength/ductility relationships via plasticity induced transformation effects is outlined.

General Abstracts: Materials Processing and Manufacturing Division: Forming and Machining

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

Thursday AM Room: 606
February 18, 2010 Location: Washington State Convention Center

Session Chair: To Be Announced

8:30 AM
Effect of AWJ Machining Processes on Flexural Properties of CFRP Composites: *T. Briggs*[1]; M. Ramulu[1]; [1]University of Washington

This paper investigates the dependence of mechanical performance on the manufacturing process chosen to prepare composite material testing specimens. Carbon Fiber Reinforced Plastic (CFRP) specimens have been machined from consolidated plates to testing coupons using abrasive waterjet (AWJ) cutting as well as abrasive diamond saw (ADS) cutting. The extensional and flexural properties of the CFRP composite material system have been experimentally determined through tensile and 3-point bend testing, respectively. The measured, in-plane elastic properties, in addition to micro and macroscopic features, failure loads and damage progression behavior, have been shown to have a correlation to the surface topography induced by the respective post processing operation.

8:50 AM
A Simple Method for Producing Large Tubular Components of Varying Profiles: *Michel Guillot*[1]; Augustin Gakwaya[1]; Xavier Elie-dit-Cosaque[1]; [1]Laval University

Aluminum tubes of varying profiles are used for structural components in automobiles, bicycles and many products. Because tubular hydroforming can be very expensive for large components, an alternative technique that can produce many simple shapes (e.g. rectangular, L, …) without internal pressure is introduced. The technique involves dies which internal geometry is defined such as to provoke during die closing, a forming sequence which result into the desired shape after springback.First, the paper presents this forming technique, tooling and the computational method used to establish the shape of the die and tool motion for a given final geometry. Different shapes are tabulated for AL6061-O and T6 using extruded 50.8mm O.D. tubes. Thereafter, tests are carried out (1) in straight tubes of constant section profiles, (2) in straight tubes of varying section profiles, and (3), in bent tubes of constant section profiles. The resulting components are characterized dimensionally and metallurgically.

9:10 AM
A Study of Electromagnetic Compression of Thin-Walled Steel and Aluminum Tubes: *Anupam Vivek*[1]; Keun-Hwan KIM[2]; Glenn Daehn[1]; [1]Ohio State University; [2]POSCO

Electromagnetic forming represents an elegant and efficient way of reducing tube diameter as there is no physical contact with the tube and deformation can be much more stable because of inertial stabilization of buckling. The ease and precision for controlling pressure is a major advantage of this technique and hence small to large tubes can be compressed using the same basic equipment. Velocity, displacement, currents and strains are measured with high accuracy and resolution using advanced instrumentation like Photon Doppler Velocimetry and Rogowski coils. In this work, Steel and Aluminum tubes are electromagnetically compressed and experimental results are compared to a numerical model. The model could not predict the buckling so it is experimentally studied in detail by varying material temper, energy level and pressure rise time. All the experimental and simulation results will be presented and subsequently discussed.

9:30 AM
Texture Control for Improving Deep Drawability of Cu Bearing New BH Steel: *Kyu Hwan Oh*[1]; Dong Nyung Lee[1]; Yang Mo Koo[1]; Se Min Park[1]; Sung-il Kim[1]; [1]Graduate Institute of Ferrous Technology, Pohang University of Science and Technology

The deep drawability, e.g., the limiting drawing ratio or the plastic strain ratio, of steel sheets is well known to increase with increasing density of γ fiber (<111>//ND with ND denoting the sheet normal direction) component in their textures. Therefore, steel sheets for deep drawing are desired to have as high density of γ fiber component as possible. A thermomechanical process has been developed to increase the γ fiber component in Cu bearing new BH steel manufactured by POSCO. The process comprises the first rolling of about 20% reduction and subsequent annealing at 780°C and the second rolling of about 70% reduction and subsequent annealing at 780°C. The first step process aims at seeding the γ fiber grains, which can grow preferably in the second step process. In this way the density of γ fiber component in the steel sheet substantially increased compared with that in the conventionally processed one.

9:50 AM
Edge Cracking Characterization and Analysis on Advanced Dual Phase Steels: *Xin Wu*[1]; [1]Wayne State University

Advanced high strength dual phase steels have been applied for lightweight structures such as automotive bodies. One of the challenges is its sensitivity to edge cracking and the uncertainty to predicting the stamping failure. In this paper material microstructures are characterized, and the edge fracture as a function of material grade, orientation and deformation histories are examined, and the mechanisms responsible for edge fracture is determined. Mechanical analysis is performed using a meso-scale composite model to reflect various dual phase microstructural features and the response to the deformation and fracture.

10:10 AM
Closure of Cylindrical Voids in a Slab under Plane-Strain Compression: Jong Jin Park[1]; *Jae Won Lee*[1]; [1]Hongik University

Voids in a slab or an ingot are required to be closed during rolling or forging processes. However, the level of closure depends on the location of a void since the state of stress is inhomogeneous. In the present study, cylindrical voids were assumed to be located along the thickness direction in a slab that was under plane-strain compression along the width, and the closure phenomenon of the voids was investigated by experiment and numerical analysis. It was found that a void is closed through contraction and collapse stages, where it deforms to an ellipse and folds along the major axis, respectively. It was also found that a void is closed when the effective strain reaches a certain value, which in fact depends on the aspect ratio of the cross section of a void but not on its magnitude.

10:30 AM Break

10:50 AM
Springback Correction by Electromagnetic Deformation in Sheet Metal Fabrication: *Jianhui Shang*[1]; Steve Hatkevich[1]; Larry Wilkerson[1]; Jeremy Westerheide[1]; Allen Jones[1]; [1]American Trim LLC

Springback is caused by the elastic recovery of bending area after unloading. It leads to the deviation of part shape. Therefore, springback control is a key to get the desired shape in sheet metal forming. In this study, electromagnetic forming was applied to springback correction as a second step after bending. Basic principle is to place magnetic impulses at bending area of metal parts to eliminate springback. From this principle, two approaches (direct and indirect approach) were investigated for springback correction of V-shape bent metal parts. The tested materials included Al alloy and high strength steel (HSS). The detailed experiment design and results will be presented here. Overall this study demonstrates the feasibility of springback correction by electromagnetic forming.

11:10 AM
Microstructure Evolution and Static Re-Crystallization Kinetics of High Manganese Steel at Hot Rolling Conditions: *Hyukjin An*[1]; Soon Gi Lee[2]; Jong-Kyo Choi[2]; Jae-Sang Lee[1]; Yang-Mo Koo[1]; [1]POSTECH; [2]POSCO

To study the static re-crystallization under the hot rolling conditions of high manganese steel, double compression isothermal tests and multi-pass hot torsion tests were performed. It is important to estimate austenite microstructure depending on hot rolling condition, for controlling final mechanical properties.

It is known that Tnr corresponds to the temperature where re-crystallization starts to be incomplete. But actually the "pancake" structure, the standard no re-crystallization microstructure on rolled microstructure, appears at lower temperature than Tnr. Thus, in order to estimate austenite microstructure, the observed austenite aspect ratio are compared with softening fraction between Tnr and RST (re-crystallization stop temperature) has been designed. No-recrystallization temperature (Tnr) was measured by using multi-pass continuous cooling torsion tests. RST and RLT(re-crystallization limit temperature) was calculated from softening ratio which is measured by using double deformation tests.

11:30 AM
New High Strength Ductile Bainitic Forging Steels: *Christoph Keul*[1]; Marcus Urban[2]; Martin Fischer[1]; Gerhard Hirt[2]; Wolfgang Bleck[1]; [1]Institute of Ferrous Metallurgy; [2]Institute of Metal Forming

New alloying and process designs without a secondary heat treatment are necessary to enable an economic production of forged steel components that combine high strength and good toughness. Forging steels containing approx. 0.20%C, 1.5%Si, 1.5%Mn, 1.3%Cr, 0.0025%B, 0.03%Nb, 0.02%Ti have been found adequate to achieve these aims. This alloying concept, combined with an adapted process route, enables a bainitic microstructure which leads to a tensile strength greater than 1200MPa, a total elongation greater than 10% and a toughness bigger than 27J at room temperature. These material properties have been accomplished by a defined deformation/heat treatment concept tested in laboratory and have been verified in industrial scale. The required bainitic microstructure formed either during a continuous or isothermal phase transformation has been characterized on a detailed morphological basis depending on the forging/cooling procedure. Therefore, a quantitative correlation between processing route and resulting mechanical properties is possible.

11:50 AM
Superplastic Blow Forming of Steel and Titanium Alloys for Aerospace Parts: *Ho-Sung Lee*[1]; Jong-Hoon Yoon[1]; Yeong-Moo Lee[1]; [1]Korea Aerospace Research Institute

By using superplastic blow forming technology, it is possible to form a complex shape in one piece with least amount of waste during machining. The present study constructs an analysis model to predict blow forming behavior of duplex steel and titanium alloy from results of biaxial and uniaxial tension tests. The experimental results show a complex shape was successfully formed from bonded sheets of superplastic metals. The results demonstrate that the developed technology to process design of high temperature blow forming by the finite element method can be applied for near net shape forming of a combustion chamber skin and a cylindrical hollow tank of ramjet engine.

12:10 PM
Cooling Behavior of Lead-Free Bismuth Bronze Produced through the Frozen Mold Casting Process: *Shuji Tada*[1]; Hiroyuki Nakayama[1]; Toshiyuki Nishio[1]; Keizo Kobayashi[1]; [1]National Institute of Advanced Industrial Science and Technology

Lead-free bismuth bronze castings were produced by several frozen molds. The effect of sand characteristics constructing frozen mold on the cooling behavior of bronze castings was examined. The sand particle characteristics such as higher thermal conductivity, greater grain size and spherical shape increased the cooling rate of castings. The cooling potential of frozen mold relates closely to the behavior of vaporized water. In the frozen mold, the ice near the mold surface contacting to molten metal thaws immediately and changes to vapor just after pouring. Then it blows out from the mold with removing the heat from the casting. Accordingly, the frozen mold which has good air permeability is able to enhance its cooling ability. The structure of lead-free bismuth bronze castings was successfully refined by the frozen mold casting process, which enabled to accelerate the cooling rate of cast products drastically.

General Abstracts: Structural Materials Division: Environmental Degradation

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

Thursday AM — Room: 601
February 18, 2010 — Location: Washington State Convention Center

Session Chair: To Be Announced

8:30 AM
Phase Field Modeling of Sintering Process in Thermal Barrier Coating Systems: *Anter El-Azab*[1]; Jie Deng[1]; Karim Ahamed[1]; [1]Florida State University

The development of thermal barrier coating (TBC) systems with well controlled and predictable performance is crucial for making breakthroughs in many high-temperature application areas. Related research and development efforts, however, have been highly experimentally oriented and little modeling effort is being conducted in parallel to understand the complex nature of bonding and failure mechanisms in TBC systems. At the root of these failure mechanisms is the interlayer and surface diffusion driven by high temperature, stress gradients and chemical composition differences between different components of the TBC systems. In this presentation we will discuss the critical aspects of connection between diffusional processes, microstructural and morphological changes and sintering mechanisms in TBC systems, and present phase field modeling results for the densification and porosity changes and inter-layer diffusion in typical TBC systems.

8:50 AM
High-Temperature Cyclic Oxidation of Pd/Pt-Modified Nial Bond Coats: *Raghavendra Adharapurapu*[1]; Dan Widrevitz[1]; Jun Zhu[1]; Don Lipkin[2]; Voroman Dheeradhada[2]; Tresa Pollock[1]; [1]University of Michigan; [2]General Electric (GRC)

Oxidation resistant NiAl-based bond coats are an important element of thermal barrier coating systems. A combinatorial approach to investigating the effects of higher order additions to NiAl, including Pt, Pd and Hf, on the oxidation and interdiffusion behavior of the bond coats has been developed. Bond coats with compositions in the range of Ni-(33-39)Al-5Cr-(2-8)Pd/Pt were deposited on RenéN5 substrates. Long-term cyclic-oxidation experiments on Pd/Pt-modified NiAl+Hf at 1100°C revealed similar oxidation kinetics in both type of coatings. While the alumina scales formed on Pd-modified bond coats were slightly thicker than the Pt-modified ones, both exhibited a high resistance to large-scale spalling. Microprobe measurements have also shown that the difference in the penetration depths of Pd and Pt into the substrate are not as large as expected from the higher interdiffusion-coefficient of Pd in NiAl/Ni. SEM and XRD analysis of the oxidation products at various stages of oxidation will be presented.

9:10 AM
Role of TM (TM = Pd, Rh, Ir) on Stability and Oxidation Behavior of Ternary β-NiAl: *Travis Brammer*[1]; Pratik Ray[1]; Yi Ye[2]; Matthew Kramer[2]; Mufit Akinc[1]; [1]Iowa State University; [2]Ames Laboratory

The drive for greater efficiencies and clean power generation requires the modern day gas turbines to operate at as high a temperature as possible in harsh operating conditions. Controlling oxidation at these elevated temperatures is a prime concern for system lifetime. In our work, we focus on the \946-NiAl. Choice of alloying additions for the current work was made using a multi-stage 'sieving process' to reduce the large number of potential alloying elements. Initial filtering of the prospective elements was done using extended Miedema model. Promising elements were studied within the framework of

DFT using VASP to check the role of minor additions on stability. Pd, Rh and Ir were deemed the most suitable for experimental testing. Additionally, the oxidation behavior of NiAl has been analyzed as functions of composition and temperature. The alloys were tested at isothermal temperatures ranging from 1100°C-1300°C, and thermal cycling at 1150°C.

9:30 AM
Investigation of the Stress Corrosion Cracking of Carbon Steel in Fuel Grade Ethanol Environments: *Lindsey Goodman*[1]; Xiaoyuan Lou[1]; Preet Singh[1]; [1]Georgia Institute of Technology

Recently, there has been much evidence of the phenomenon of stress corrosion cracking (SCC) in steel equipment in the ethanol industry. Research shows the effects of simulated fuel grade ethanol (SFGE) and impurities such as water, chlorides, and pH_e on SCC severity in carbon steel. In this study, carbon steel was exposed to fuel grade ethanol (FGE) to concurrently investigate surface film formation on carbon steel and compositional changes in the FGE environments. Ethanol breakdown can occur over time based on environmental conditions, thus effects of these compositional variations on carbon steel surfaces were investigated. Scanning electron microscopy (SEM), and X-ray diffraction (XRD) were used to characterize the steel surface. Raman spectroscopy was used to characterize both FGE chemical composition and steel surface. Electrochemical behavior of carbon steel in the ethanol environments was evaluated. Experimental results are detailed in the body of the paper.

9:50 AM
Observation and Detection of Corrosion on Aerospace Bearing Steels in Ester Based Lubricants: *Michael Hurley*[1]; Cole Smith[1]; Darryl Butt[1]; [1]Boise State University

Lubricant degradation or contamination in jet turbine engines is a precursor to corrosion of the bearing materials. Once corrosion is initiated, the eventual outcomes are decreased engine performance, required service, and parts replacement. Characterization of the bearing steel corrosion behavior in the engine environment is elusive since typical electrochemical corrosion measurements are ineffective due to ultra high solution resistance of the lubricating fluid. In this work EIS (Electrochemical Impedance Spectroscopy) and in-situ optical microscopy were utilized in an effort to characterize the corrosion behavior of M50 and P675 bearing steels tested in a range of water and chloride contaminated ester based oils. EIS was found to be sensitive to water contamination levels and relatively insensitive to chloride contamination level and the presence of active corrosion. Further insight in to the corrosion behavior was obtained via optical microscopy of the complex interaction of water, oil, and steel microstructure in-situ.

10:10 AM Break

10:20 AM
Assessment of Slag-Aided Deoxidation Process in 3.5crmov Rotor Steel: *June-Seong Park*[1]; Chang-Woo Seo[1]; Seonhyo Kim[1]; [1]POSTECH

Refining process of rotor steels by applying slag-aided deoxidation using $CaO\text{-}CaF_2$ flux has been investigated at 1873K. Initial deoxidation rate was faster through increasing CaF_2/CaO ratio until 1.15. However, experimental results recommended 1:1 to optimum CaF_2/CaO ratio because excess CaF2 contents promoted the dissolution of MgO at the crucible. By considering slag-aided deoxidation, the Deoxidation rate is decreased with increment of Fe_tO. At input of Ca-Si deoxidant for slag deoxidation, Silicon acted not only Ca-carrier and slag reductant, but also affected the direct deoxidation of molten steel. 3% of Ca-Si deoxidant was insufficient in slag with 5% of Fe_tO. 7% of Ca-Si deoxidant affected adversely by increasing silicon content, and deoxidation rate was similar to input 5%. Thus effective content was 5% of Ca-Si deoxidant.

10:40 AM
Factors Affecting the Environmental Assisted Cracking Behavior of 2205 Duplex Stainless Steel: *Kevin Chasse*[1]; Di Yang[2]; Preet M. Singh[1]; Richard W. Neu[3]; [1]Georgia Institute of Technology; [2]University of Colorado at Boulder; [3]Georgia Institute of Technology and University of Colorado at Boulder

The reliable performance of duplex stainless steels (DSSs) in chloride- and sulfide-containing solutions is important to many industrial processes. Previous studies have shown that DSSs are susceptible to environmental assisted cracking (EAC) under certain conditions in these solutions; however, the mechanical and electrochemical conditions under which DSSs may become susceptible are not well understood. To elucidate some of these mechanical and electrochemical conditions, the EAC susceptibilities of a 2205 DSS were evaluated in an acidic-chloride solution and a sulfide-containing caustic solution. Low frequency cyclic tests were performed for a fixed number of cycles, and the crack initiation events were examined after these tests. In the chloride solution, corrosion pits are the preferential sites for crack initiation under cyclic loading. In the sulfide-containing caustic solution, precipitates tend to be the preferential sites for cracks to initiate, especially the ones at or near the interface of the phase boundary and grain boundary. Hydrogen embrittlement (HE) was also found to be a potential form of EAC in this solution at room temperature when a cathodic potential (CP) was applied.

11:00 AM
Hydrogen Embrittlement of a Bainitic Wheel Steel: *Ren Xuechong*[1]; Liu Fenbin[1]; Su Yanjing[1]; Chu Wuyang[1]; [1]University of Science and Technology Beijing

The slow strain rate tensile (SSRT) test and hydrogen-induced delayed cracking (HIDC) were investigated in a noval bainitic wheel steel. The results showed that hydrogen embrittlement susceptibility of the bainitic wheel steel was really higher than that of ferrite-pearlite wheel steel. The threshold stress intensity factor of hydrogen-induced delayed cracking, KIH, decreased exponentially with the increasing of diffusible hydrogen concentration C0. And the crack propagating rate can achieve as high as 0.2 mm/min when C0=1.6×10-6.

11:20 AM
Microstructural and Mechanical Aspects of High Nitrogen Steels at Cryogenic Temperature: *Zurui Zhang*[1]; Huabing Li[1]; Zhouhua Jiang[1]; Zhen Li[1]; [1]Northeastern University

Charpy V-Notch impact tests of high nitrogen austenitic stainless steels with different nitrogen concentration 0.96, 0.88 and 0.82 (wt. %) from 77K to 293K are processed in this paper. The fracture facets are observed by using scanning electron microscopy (SEM) and transmission electron microscopy (TEM) to reveal the micro fracture mechanism. With increasing the nitrogen content, the ductile to brittle transition temperature (DBTT) increases. The change of fracture patterns of high nitrogen austenitic stainless steels is dimple==>shallow dimple==>mixture of quasi-cleavage facets and dimple==>cleavage facet. Fracture facets with river patterns or tear ridges, along annealing twin boundary and cross the annealing twin plane are observed in this investigation. Critical dislocation density around crack-tip field $\rho_c=(6\pi\tau_p^2/K_{Ic}^2)^2$ can be used for explaining DBT behavior at cryogenic temperature. Deformation twinning is frequently observed at cryogenic temperature. Crack forms along the coherent twin boundary between twinning and the matrix.

11:40 AM
The Relationship between Sliding-Wear Rate and the Microstructure of AISI 1020 Plain-Carbon Steel: Jong Chul Kim[1]; Jun Ki Park[1]; Sul Ki Yi[1]; *Yong-Suk Kim*[1]; [1]Kookmin University

The relationship between sliding-wear rate and the microstructure of plain-carbon steel (0.2C-0.7Mn-0.05Si) was investigated. The steel was heat treated under various conditions to have different microstructures, and the effect of microstructure on the sliding wear was explored. Dry sliding wear tests of the heat-treated steel were carried out using a pin-on-disk wear tester at a fixed load of 100 N at room temperature. AISI 52100 bearing steel and alumina balls were employed as a counterpart. Tensile properties and hardness of the heat treated steel were evaluated to characterize wear behavior of the steel. The wear rate of the steel heat treated under different conditions did not change significantly with the microstructural variation, though hardness of the steel varied significantly with the microstructure. Effects of the morphology and volume fraction of constituting phases of the microstructure on the wear rate were explored in connection with deformation beneath wearing surface (subsurface-deformation-layer formation).

12:00 PM
Dynamic Tensile Extrusion Behavior of DU and U6NB: *Carl Trujillo*[1]; George Gray[1]; Ellen Cerreta[1]; Joel Montalvo[1]; Daniel Martinez[1]; [1]Los Alamos National Laboratory

While there have been studies investigating the quasi-static, stress-strain behavior of uranium alloys, there have been few studies that have examined the high strain, high strain rate response of these materials. One way to examine this behavior is through high-rate, tensile extrusion. Using a technique developed at Los Alamos National Laboratory, U6Nb and DU spheres were accelerated to velocities of 550m/s and extruded through a steel die. High speed photography captured the in-situ extrusion response. Recovered fragments were characterized using optical and electron microscopy. Spheres were fired at temperatures ranging from 25-300C. At quasi-static rates, DU and U6Nb display ductile behavior. However, during high strain rate extrusion, deformation was dominated by shear processes that significantly limited ductility. Comparisons between the temperatures and extrusion rates will be presented. Continuum simulations based on Mechanical Threshold Stress (MTS) models will be performed to provide insight into the dynamic extrusion process.

Jim Evans Honorary Symposium: Beyond Berkeley Times

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

Thursday AM Room: 620
February 18, 2010 Location: Washington State Convention Center

Session Chair: Ben Li, University of Michigan

8:30 AM Introductory Comments

8:40 AM
Contamination Issues – A Contrast in Industries: *Stanley Siu*[1]; [1]S & V Siu Associates, LLC

Contamination issues in the semiconductor industry have always been a major focus of attention due to its direct impact on device performance and yield. The term "killer defects" is indicative of the seriousness of this issue and sophisticated technologies to detect contaminates have evolved to such a level that contamination and defect detection has become an industry in itself. In the medical device industry contamination has received much less attention, but as devices have become more sophisticated, this issue is beginning to gain more attention. The medical device industry is now venturing into the realm of metrology that has traditionally been the territory of semiconductor processing. Major differences in goals, objectives, and requirements make contamination detection and mitigation a very different and challenging problem and will be highlighted with a case study in this paper.

9:05 AM
Electrodynamic and Thermal Interaction of Nanoparticles in Hyperthermia Cancer Therapy and Solar Energy Systems: *Ben Li*[1]; [1]University of Michigan

The paper presents a study on the electrodynamic and thermal interaction of nanoparticles as applied to therapeutic treatment of cancer patients and to development of high efficiency solar energy systems. For these applications, nanoparticles need to have a structure that is tunable to a given frequency of an electromagnetic energy source for resonance absorption and/or scattering. Electrodynamic model is developed based on the analytical and numerical solution of the full 3-D Maxwell equations to determine the tunable resonance absorption as a function of varying structure parameters. The electromagnetic model is then linked to a thermal model, which is based on the solution of combined internal thermal radiation, conduction and convection. Experiments are conducted to validate the electromagnetic and thermal models. Both modeling and experimental results will be presented for the systems under consideration for cancer treatment and solar energy system applications.

9:30 AM
Metallurgical Design Issues at Cirque du Soleil: *Daniel Cook*[1]; [1]University of Nevada, Las Vegas

The modern live entertainment industry poses a number of interesting engineering problems in the design and use of large, dynamic, theatrical stage components, which can be on the order of 10s of meters in length and 100s of metric tons in moving mass. A prime example of these types of stage components can be seen at the Cirque du Soleil show Ka. Since show opening in 2005, a number of the components of the Gantry Lift, the main stage system, have needed modification to correct operational issues that arose from the initial design(s). This paper will focus on how mathematical modeling and analysis of the as-built components has been conducted to correct and improve operation of the stage system. In particular, this paper will describe the static and dynamic structural calculations which have been used as the basis for component redesign to alleviate fatigue failure in the stage system.

9:55 AM
An Electrochemical Technique for Minimizing Soil and Ground Water Contamination by Heavy Metals Leached from Solid Industrial Wastes: Nilesh Shukla[1]; Manoj Harbola[1]; Kali Sanjay[2]; *Rajiv Shekhar*[1]; [1]Indian Institute of Technology; [2]Institute of Minerals & Materials Technology

Indiscriminate dumping of solid industrial wastes in un-engineered sites and the consequent soil and water contamination by heavy metals -- dissolved in rain water -- is a major environmental hazard in India. This study addresses an important issue: how do we minimize the rain water assisted transport of toxic heavy metals from solid wastes to the ground water? Preliminary experiments have shown that electrochemical fencing, which uses an electric field to capture the heavy metal ions, is a viable technique for slowing down the rain-assisted transport of heavy metals through soil. Experiments simulating the natural rain fall conditions on a saturated soil covered with a dichromate residue have been carried out. The effect of applied voltage, electrode depth, and electrode configuration on the efficacy of electrochemical fencing has been investigated. A mathematical model that calculates the trajectory of Cr(VI) ions to predict the efficacy of electrochemical fencing has been formulated.

10:20 AM Break

10:35 AM
Hall Cell MHD Instability: Recent Theoretical Analyses and Experimental Support: *Donald Ziegler*[1]; [1]Alcoa Primary Metals

We review progress on understanding of MHD instability in Hall cells. Recent theoretical work has shown the existence of other types of instability beyond the classical caused by the vertical component of the magnetic field. In this work, we describe our calculations of one of these instabilities and show evidence from plants that appear to fit the phenomenon described by the theoretical work.

11:00 AM
Common Modeling Approaches in Displays: Case Studies in Organic Light Emitting Diodes and Plasma Display Panels: *Deepak*[1]; [1]IIT Kanpur

The design of electronic devices that are based on current flow is commonly described by a drift-diffusion type approach, which received prominence with its use in design of silicon based electronic devices. This paper addresses the use of same approach in displays: the plasma display panels (PDPs) and organic light emitting diodes (OLEDs). While the drift-diffusion approach is the same in both, in PDP, new physics is included through plasma reactions that create the charged and excited species in gas and innovative boundary conditions. In OLEDs, however, the physics is entirely different from inorganic semiconductors due to hopping transport of charges and the excitons that play a prominent role. However, the approach of drift-diffusion is so ubiquitous that attempt is still made to cast the problem in that form. Using these approaches, we demonstrate both the principle of operation and design of devices in PDPs and OLEDs.

11:25 AM
Modeling Pulsatile Blood Flow in End-to-Side Anastomoses: *Daniel Cook*[1]; Christopher Thompson[2]; [1]University of Nevada, Las Vegas; [2]General Electric

Analysis of the transient, pulsatile blood flow in a simplified anastomosis located between the human aorta and a centrifugal heart assist pump was carried out. Modeling efforts focused on the fluid flow in the anastomosis for junction angles of 60, 75, and 90 degrees at varying heart and pump flow rates. Results from this modeling indicated that higher junction angles produced larger areas of stagnation and shear gradients internal to the fluid, whereas lower junction angles yielded higher shear rates at the arterial wall opposite to the junction.

Magnesium Technology 2010: Forming and Welding

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

Thursday AM — Room: 613
February 18, 2010 — Location: Washington State Convention Center

Session Chairs: Amit Ghosh, University of Michigan; Jon Carter, GM R&D

8:30 AM
Test Results and FEA Predictions from Magnesium AZ31 Sheet Beams in Bending and Axial Compression: *David Wagner*[1]; Stephen Logan[2]; Kathy Wang[3]; Tim Skszek[4]; [1]Ford Motor Company; [2]Chrysler LLC; [3]General Motors Corp.; [4]Magna Cosma International

Load versus displacement measurements are compared to finite element analysis (FEA) predictions for magnesium AZ31 sheet beams. The beams are two stampings joined with epoxy and rivets. The longitudinal axis of the beams is aligned in the rolling direction in some samples and in the transverse direction in others. Results from quasi-static four-point bend, quasi-static axial compression and high-speed axial compression tests of AZ31 sheet beams show the beam's behavior over a range of loadings and the two orientations. The AZ31 beams exhibit significant material cracking and splitting in all tests. LS-DYNA material model MAT_124 captures the sheet magnesium AZ31 constitutive behavior over a range of strain rates and accommodates different responses in tension and compression. The boundary conditions in the FEA predictions closely mimic the loading and constraint conditions in the component testing. LS-DYNA explicit FEA predictions of the tests agree to differing degrees with the test results.

8:50 AM
Microstructure and Mechanical Properties of Magnesium Extrusion Alloys AM30 and AZ31: *Alan Luo*[1]; Joy Forsmark[2]; Xichen Sun[3]; Scott Shook[4]; W.Z. Misiolek[5]; Raj Mishra[1]; [1]General Motors Corporation; [2]Ford Motor Company; [3]Chrysler Group LLC; [4]Timminco Metals; [5]Lehigh University

Magnesium alloy extrusions offer potentially more mass savings compared to magnesium castings in lightweighting vehicle structures applications. The objective of the United States Automotive Materials Partnership (USAMP) "Magnesium Front End Research and Development" (MFERD) project is to evaluate various magnesium alloys for automotive body applications. As a task in the MFERD project, solid and hollow extrusions of AM30 and AZ31 alloys were fully characterized for grain structure and crystallographic texture. Mechanical properties in tension and compression were tested in extrusion, transverse and 45 degree directions. Mechanical properties of magnesium extrusions are generally better than those of conventional die cast alloys. Significant tension-compression asymmetry (different yield strength in tension and compression) and plastic anisotropy (different plastic behavior in different directions) are due to the strong texture developed in the extrusion process.

9:10 AM
Texture Development in a Twin Roll Cast and Warm Rolled ZK60 Magnesium Alloy: *Hongmei Chen*[1]; Huashun Yu[2]; Suk Bong Kang[3]; Guanghui Min[2]; [1]Jiangsu University of Science and Technology; [2]Shandong University; [3]Korea Institute of Materials Science

The effect of rolling conditions on the microstructure and texture development of twin roll cast ZK60 alloy strip was investigated. Texture of ZK60 Mg alloy sheets were evaluated by X-ray diffraction method in this study. Tensile test was performed to show the influence of the per pass thickness reduction on mechanical properties. The microstructure of ZK60 alloy sheets consisted of fibrous structure with elongated grains and a relatively density of shear bands along the rolling direction which were warm rolled at 350°C with 10%, 30% and 50% thickness reduction per pass. Dynamic recrystallization could be found during the warm rolling process with different per pass thickness reduction. Grain refinement was found to occur during the warm rolling process, producing a finer grain size of which was warm rolled with 50% reduction in single pass rolling at 350°C. This could result in better mechanical properties.

9:30 AM
Cruciform Geometries for Elevated Temperature Biaxial Testing of Mg AZ31B: Fadi Abu-Farha[1]; *Louis Hector Jr*[2]; [1]Pennsylvania State University; [2]GM R&D Center

Plastic deformation of metals is typically characterised with the uniaxial tensile test. However, multiaxial loading in sheet metal forming requires more complex tests such as the controlled biaxial test with cruciform specimens. Efforts have been limited by testing instrumentation complexity, especially at higher-than-ambient temperatures, and specimen designs that preclude plastic strain accumulation in the gauge section. Here, focus is on development of Mg AZ31B cruciform geometries where plastic deformation is achieved in the gauge section. Testing was conducted in a biaxial apparatus capable of multi-rate stretching at temperatures up to 500 °C. Deformation of the gauge section of each specimen during loading to fracture was recorded with digital images at a constant rate. A state-of-the-art digital image correlation algorithm was then applied to compute strain fields from the images. The results provide key insights into the influences of specific geometrical parameters on the degree of deformation-biaxiality in a cruciform specimen.

9:50 AM
Characterization of Continuous-Cast AZ31B Magnesium Alloy Sheets and Lubricants for Warm-Forming - Friction Effects: *Aashish Rohatgi*[1]; Darrell Herling[1]; Eric Nyberg[1]; [1]Pacific Northwest National Laboratory

Our goal is to understand the inter-relationships between the initial properties of continuous-cast magnesium alloy (AZ31B) sheets and their subsequent formability and post-formed mechanical performance for use in cost-effective, lightweight, automotive body panels. As-received sheets, provided by the AMD 602 team, have been characterized by surface roughness measurements using mechanical and optical profilometry. Microstructural analysis of as-received sheets and formed pans is being performed via optical microscopy, electron backscattered diffraction (EBSD) and microhardness measurements. Mechanical properties of AZ31B pans are being characterized by room-temperature quasi-static tensile tests. Several commercial lubricants are being evaluated by elevated temperature friction tests and will be used to conduct limited dome height (LDH) tests on as-received sheets. This research will identify how starting properties of continuous-cast AZ31B sheets could be controlled to achieve an optimum combination of formability and post-formed mechanical performance to enable their use as a low-cost alternative to conventional wrought AZ31B sheets.

10:10 AM Break

10:30 AM
High Strength ZK60 Mg Plate Produced by Grain Refinement and Precipitation during Alternate Biaxial Reverse Corrugation (ABRC) Process and Friction Stir Process (FSP): Bilal Mansoor[1]; Sibasish Mukherjee[1]; *Amit Ghosh*[1]; [1]University of Michigan

Under research support by US Army, a process of Alternate Biaxial Reverse Corrugation (ABRC) was explored to impart large severe plastic deformation to ZK60 Mg alloy. This process had previous utilized to strengthen AZ31 Mg and reported elsewhere (Yang and Ghosh). The present results with ZK60 alloy exhibit higher strength (>350 MPa), and retention of adequate ductility (> 7% tensile elongation). The enhanced strength levels are believed to be influenced by a number of precipitates found in this alloy not existing in AZ31 alloy, in addition to grain size strengthening produced by about 1-2 micron grain size. Partial depth penetration into sheet from the top and bottom surfaces of alloy by friction stir process was also examined for this alloy to cause a different form of grain refinement. The strengthening effect in this case was found to be higher.

10:50 AM
Formability of Mg Alloys at Room Temperature: *D.-W. Kim*[1]; D. H. Kang[2]; S. Kim[3]; G. T. Bae[4]; K. H. Kim[1]; Nack J. Kim[1]; [1]POSTECH; [2]McGill University; [3]General Motors R&D Center; [4]Georgia Institute of Technology

Mg alloys are the lightest commercial alloys developed so far and have great potential for high performance automotive applications. For the application of Mg sheet products, it is necessary for the sheets to be readily formable for making complicated shapes. Therefore, many researches are being carried out to enhance the high temperature formability of Mg alloy sheets. However, further improvement is certainly needed to ensure the room temperature formability of Mg alloys to expand their applications. In the present study, the relationship between the room temperature formability and the microstructural features of

Mg alloys has been investigated. Various Mg alloys with various microstructural features were fabricated by twin-roll casting and their uniaxial tensile properties were correlated with room temperature formability measured by the Erichsen cupping test. It shows that the alloys with larger work hardening capacity have the better formability at room temperature.

11:10 AM
Dynamic Blankholder Control for the Enhanced Forming Limit of Magnesium Sheets: *Wonkyu Bang*[1]; [1]RIST

The deep drawability of magnesium is known to be affected significantly not only by forming temperature and speed, but by blankhold force. Since magnesium alloys typically exhibit very weak strain hardening at the elevated temperature, thinning (instability) can be triggered by small amount of excessive blakhold force. In this study, a servo-controlled blankholder mechanism was implemented to the dies/tools for magnesium warm drawing. As reported in the previous studies of high strength steels and aluminum alloys, improvement of forming limit coupled by lower forming load was reproduced for magnesium warm forming. Cyclic 'clamp-and-release' blankholder motion eased off the resistance of metalflow from flanges to walls, which resulted in smaller stretcher strain and more uniform thickness distribution. By optimizing the control function of blankholder action, the forming limit can be increased by 20% and more.

11:30 AM
Joining Magnesium to Steel: *Yuri Hovanski*[1]; Glenn Grant[1]; Mike Santella[2]; [1]Pacific Northwest National Laboratory; [2]Oak Ridge National Laboratory

Solid state joining methods were utilized to evaluate the joining potential of magnesium alloys to automotive sheet steels. Friction stir welding, friction stir spot welding, and ultrasonic welding techniques were developed to produce structural joints between both cast and wrought magnesium components and coated and uncoated steel sheets. The effects of tool design and process parameters were evaluated. The joint interface was examined, allowing characterization of the resultant mixing and microstructure. Mechanical performance of joints produced using each solid state technology were evaluated and presented.

11:50 AM
Accumulative Roll Bonding of Wrought Magnesium Alloy: *H. Nayaka*[1]; B.S.S. Daniel[1]; G.P. Chaudhari[1]; [1]IIT Roorkee

Accumulative Roll Bonding (ARB) is a severe plastic deformation process, which can produce high strength metal alloys with ultrafine-grained structure. An ultrafine-grained AZ61 magnesium alloy was produced using upto six ARB passes at a rolling temperature of 300°C and upto three passes at a rolling temperature of 270°C. Reduction of 50% was employed for each pass. The mechanical properties are evaluated by micro-hardness tests. The micro hardness values for the as-received AZ61 alloy was found to be 60 VHN and that of six pass ARB sample was 125 VHN. Resulting ultrafine-grained microstructure was characterized by the use of optical microscopy and TEM. DSC analysis was performed to study the thermal stability of the roll-bonded samples.

12:10 PM
Mechanical Properties and Corrosion Behavior of Friction Stir Welded Mg/Mg- and Mg/Al-Joints: *Otmar Klag*[1]; Guntram Wagner[1]; Dietmar Eifler[1]; [1]Institute of Materials Science and Engineering / University of Kaiserslautern

In this research project the friction stir weldability (FSW) of similar joints of die casted AZ91-Mg-alloy, MRI-Mg-alloys and dissimilar joints between AZ91-Mg-alloy and AA5454-Al-alloy were investigated. In monotonic tensile tests for welds between similar materials tensile strengths at the value of the parent materials were determined. With two-dimensional hardness measurements it could be proved that in the case of the similar joints the FSW-process leads to a decrease of the hardness in the welding zone as a result of the of the inducted thermal energy. But for dissimilar joints an extreme increase of the hardness in the nugget was observed. SEM investigations and EDX element mappings have shown that this is caused by the formation of intermetallic phases particularly positioned as interlayers in the contact area between the Mg- and the Al-alloy. Cracks are predominantly initiated at the intermetallic phases. Furthermore the corrosion behavior of the FSW zone was investigated.

Magnesium Technology 2010: ICME II and Biomedical Applications

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

Thursday AM — Room: 612
February 18, 2010 — Location: Washington State Convention Center

Session Chairs: John Allison, Ford Motor Company; Wim Sillekens, TNO Science and Industry

8:30 AM
Two- and Three-Dimensional Cellular Automaton Models for Simulating Dendrite Morphology Evolution of Cast Magnesium Alloys: Liang Huo[1]; *Zhiqiang Han*[1]; Baicheng Liu[1]; [1]Tsinghua University

Two- and Three-dimensional cellular automaton (CA) models have been developed for simulating the dendrite morphology evolution of cast magnesium alloys. In the two-dimensional model a hexagonal mesh was used to perform CA calculation to reflect the texture of Mg alloy dendrites, and an orthogonal mesh was used to solve the solute transport equations. In the three-dimensional model the solute transport equation was also solved by using an orthogonal mesh, but the CA calculation was performed using a mesh that is defined by the hexagonal close-packed (HCP) crystal lattice. The growth kinetics of dendrite tips was determined by the difference between local equilibrium composition and local actual composition obtained by solving the solute transport equation. The models were applied to simulate equiaxed dendrite evolution and columnar dendrite growth of AZ91D Mg alloy. Permanent mold step-shaped castings were poured and metallographic examinations were carried out for validating the present models.

8:50 AM
Elemental Partitioning and Microstructure of Mg-Al-Ca-Sn Quaternary Alloys: *Jessica TerBush*[1]; Olivia Chen[1]; J.Wayne Jones[1]; Tresa Pollock[1]; [1]University of Michigan

Creep behavior in cast Mg-Al-Ca-based alloys depends strongly on precipitation and solid solution strengthening in the primary α-Mg cells. In MRI230D, the presence of Sn is believed to significantly influence the elemental segregation during solidification, which in turn can affect precipitation and solid solution strengthening. The influence of Sn on elemental partitioning during solidification has been systematically investigated for the quaternary Mg-Al-Ca-Sn alloy system using an electron microprobe technique coupled with a Scheil analysis. The addition of less than 1 wt% of Sn to Mg-5Al-3Ca causes an increase in the amount of Al and Ca in the primary α-Mg phase as compared to AX44 or AXJ530, although the increase is not as dramatic as the one observed in MRI230D. The creep behavior of two Mg-5Al-3Ca-xSn quaternary alloys is compared to that of AXJ530, MRI230D and MRI153M and the role of Sn on microstructure and subsequent creep behavior is described.

9:10 AM
Numerical Simulation of Flow-Induced Air Entrapment Defects in the High Pressure Die Casting Process: Shuai-Jun Li[1]; *Shou-Mei Xiong*[1]; Bai-Cheng Liu[1]; Mei Li[2]; John Allison[2]; [1]Tsinghua University; [2]Ford Motor Company

In current paper, a numerical method to predict the air entrapment defects in the high pressure die casting(HPDC) process is presented and the distribution of the entrapped air at the end of filling was represented by the concentration of air in the liquid metal. The time-dependent, incompressible Navier-Stokes equations were firstly solved by a fractional step algorithm to model the fluid flow during the mold filling of HPDC process. The free surfaces were calculated using the volume of fluid method. At each time step, the isolated air bubbles in the liquid metal were found and the pressure of the bubbles was updated using the ideal gas law. The concentration transport equation was applied for the calculation of the air entrapment distribution. X-ray inspection of a step-shape magnesium die casting was performed to verify the air entrapment prediction. The comparison between experimental and numerical results shows a good agreement.

9:30 AM
ESPEI: Extensible, Self-Optimizing Phase Equilibrium Infrastructure for Magnesium Alloys: *Shun-Li Shang*[1]; Yi Wang[1]; Zi-Kui Liu[1]; [1]MaterialsInformatics LLC

In order to store and use previous knowledge of thermodynamics in materials design, we develop a user-friendly, extensible, self-optimizing phase equilibrium computer program for magnesium alloys. This ESPEI program integrates first-principles data, thermodynamic data, parameter evaluation, and automation of phase diagram calculations with graphical user interface (GUI) designed with C-sharp and SQL (structured query language). We established the data infrastructure for storing input data used for thermodynamic modeling and output data for thermodynamic analysis. The storing of experimental data and parameter evaluation processes for phase diagram is unique for ESPEI. In the present work, the features of ESPEI will be demonstrated in the Mg-Al and Mg-Ni systems.

9:50 AM
Modeling Casting and Heat Treatment Effects on Microstructure in Super Vacuum Die Casting (SVDC) AZ91 Magnesium Alloy: *Mei Li*[1]; Ruijie Zhang[1]; John Allison[1]; [1]Ford Motor Company

Magnesium applications for the automotive and aerospace industry have received significant attention in recent years due to light-weight and consequent potential to reduce both fuel consumption and green house effect. Canada-China-USA three-country Magnesium Front End R&D (MFERD) program was established to explore the potential applications of magnesium alloys in automotive industry. In this program, the super vacuum die casting (SVDC) process was developed to produce the components. The SVDC offers advantages over conventional high pressure die casting (HPDC) in significantly reducing the air entrapment so that the produced magnesium castings can be heat treated. This paper describes the progress in the development of models to study the effects of casting and heat treatment process on the microstructures in SVDC AZ91 magnesium alloy. The microstructure model combined with property model will provide critical virtual tool in evaluating and optimizing the design and manufacturing process of magnesium alloy castings.

10:10 AM
First-Principles Study of Ternary Hcp Solid Solution Phases from Special Quasirandom Structures: Application to Mg-Al-X Alloys: *Dognwon Shin*[1]; Christopher Wolverton[1]; [1]Northwestern University

We have constructed ternary hcp special quasirandom structures (SQSs) whose correlation functions are close to those of the completely random hcp solid solutions. By performing first-principles DFT calculations of these SQSs, we have studied the Hf-Zr-Ti system, which exhibits hcp solubility in the entire composition range, to test the ability of constructed SQSs to mimic random hcp solid solutions. First-principles mixing energies and structural analysis show that our ternary hcp SQSs are capable of accurately predicting the properties of ternary hcp solid solutions. We further apply our ternary hcp SQSs to the Mg-Al-X (X= Si, Ti, Mn, Fe, Zn, and Zr) systems. We use our first-principles ternary mixing energies from SQSs to critically test a commonly used approximation in CALPHAD assessments, namely that of extrapolating ternary solution energetics from the constituent binary systems. We have also studied the effect of atomic vibrations on the mixing energies of hcp solid solutions.

10:30 AM Break

10:50 AM
Slip andTwinning in Mg Single Crystals: *Erica Lilleodden*[1]; Gyu Seok Kim[1]; Sangbong Yi[1]; Yuanding Huang[1]; Norbert Huber[1]; [1]GKSS Research Center

There is considerable need to develop mechanism-based material models for the deformation of Mg, due to its strong anisotropy and its importance in the development of lightweight structural materials. Unfortunately constitutive inputs for such models are critically lacking; fundamental studies of the critical stresses and strains and associated deformation mechanisms are needed. Employing the recently exploited method of microcompression testing along with EBSD and TEM characterization, we have investigated the deformation behavior of Mg single-crystals. The ability to obtain test volumes which can be subsequently fully characterized and which are absent of pre-existing twins makes this technique highly attractive. In this presentation, the results from microcompression testing will be discussed in terms of orientation-dependent slip activity and twinning mechanisms, and the role of geometric scale in the associated strain-strain relations.

11:10 AM
Assessing and Modeling the Impact of Initial Microstructure on Dynamic Recrystallization of Sheets: *Frederick Polesak*[1]; Paul Krajewski[2]; Babak Raeisinia[1]; Sean Agnew[1]; [1]University of Virginia; [2]GM

Samples of distinctly processed alloy AZ31 sheets were deformed in tension under strain rate and temperature conditions typical of warm forming operations. The flow curves, r-values, crystallographic texture, and metallographic observations of the microstructure were used to characterize the dynamic recrystallization behavior. Samples with larger grain sizes are shown to flow at higher stresses and undergo dynamic recrystallization more slowly than the initially fine grained samples. For samples with initially sharp basal textures, the r-value decreases when dynamic recrystallization is active. The crystallographic texture itself shows a distinct evolution during deformation involving extensive dynamic recrystallization from that observed at lower temperatures. These distinctions in r-value and texture evolution are both related to the activities of deformation mechanisms that sustain the strain. Modeling of the material flow and microstructure evolution using a viscoplastic self-consistent code is discussed.

11:30 AM
Modified AZ80 Magnesium Alloys for Biomedical Applications: *Muge Erinc*[1]; [1]TNO

Our research focuses on developing cardiovascular stent materials from magnesium alloys that satisfy mechanical and chemical requirements to be used in the human body. High aluminium alloys (7-8.5 wt %) modified with zinc, manganese, rare-earth elements and yttrium are developed by casting and thixomolding. Refining the grain size by forming is essential since zirconium is not biocompatible. It is shown that, finer grain sizes can be achieved by a single extrusion step from a thixomolded structure. Further, chemical homogeneity and solidification structure can be controlled at a higher level by thixomolding. The mechanical performance of the tubes are evaluated by tensile, compressive and torsion tests. The in-vivo biodegradation and potential inflammatory behaviour is analyzed in a mouse model by subcutaneous and intraperitoneal positioning. In-vitro tests are performed in simulated body fluid. It is shown that AE route magnesium alloys produced by thixomolding satisfy criteria concerning mechanical performance, biodegradability and biocompatibility.

11:50 AM
The Dissolution Behavior of a Mg-Zn-Ca Alloy for Biomedical Applications: *Michele Manuel*[1]; Harpreet Brar[1]; [1]University of Florida

Traditional metallic-based implantable biomaterials like stainless steel, cobalt-chromium and titanium alloys have been used for many years in structural implants for load bearing applications. These materials are considered permanent in nature and additional surgeries are needed for their removal when used in temporary implant applications like bone fixation devices. Hence, there is a need for metallic-based materials that can provide temporary structural support but yet are biodegradable and bioabsorbable after the healing process. In recent years, there has been an increase in research and development of magnesium-based alloys due to their biodegradable and biocompatible properties. This paper analyzes the dissolution behavior of a magnesium-zinc-calcium alloy in Hank's solution and the effect of surface treatment on the dissolution rate.

12:10 PM
Controlling the Biodegradation Rate of Magnesium-Based Implants through Surface Nanocrystallization Induced by Cryogenic Machining: *Z. Pu*[1]; D. Puleo[1]; O.W. Dillon, Jr.[1]; I.S. Jawahir[1]; [1]University of Kentucky

Magnesium alloys are emerging as a new class of biodegradable implant materials for internal bone fixation. They provide good temporary fixation and do not need to be removed after healing, providing the relief to the patients. However, premature failure of these implants often occurs due to high biodegradation rate caused by low corrosion resistance of magnesium alloys in physiological environments. To control biodegradation/corrosion of magnesium alloys, grain refinement on the surface was achieved through machining-induced severe plastic deformation. Liquid nitrogen was used during machining to suppress grain growth. Nanocrystallized layers with various grain size and thickness have been fabricated by controlling the machining conditions. In vitro corrosion tests proved that the nanocrystallized layers enhanced corrosion resistance to different extents, depending on the thickness and grain sizes of the layer. By proper selection of machining conditions, magnesium-based implants with customized biodegradation rates for different medical requirements can be manufactured.

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

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

Thursday AM Room: 212
February 18, 2010 Location: Washington State Convention Center

Session Chairs: Jeffrey Hawk, U.S. Department of Energy; Xingbo Liu, West Virginia University

8:30 AM Invited
Nanostructured Functional Materials for Energy Conversion and Storage: *Donghai Wang*[1]; [1]Penn State University

The role of nanostructured materials in addressing the challenges in energy has attracted wide attention. Many promising results of nanostructured materials in renewable energy harvesting, conversion and storage have demonstrated the important role of high surface area to maximize the surface activity, and the importance of optimum dimension and architecture, controlled pore channels and alignment of the nanocrystalline phase to optimize transport of electrons, ion and other species for better performance. In my talk, I will present some works on synthesis of nanostructured materials. I will also discuss how such controlled nanostructures can be used in energy conversion and storage and improve device performance for Li-ion batteries and fuel cells. Specifically, the electrochemically active material/graphene hybrid nanostructures have been studied as electrodes in Li ion battery and fuel cells showing superior capacity retention and high rate performance during lithiation/delithiation and enhanced stability as cathode catalysts for PEM fuel cells.

9:10 AM
Cathode/Anode Selection and Full Cell Performance for Stationary Li-Ion Battery System: *Daiwon Choi*[1]; Donghai Wang[2]; Vilayanur Viswanathan[1]; Wu Xu[1]; Ji-Guang Zhang[1]; Gary Yang[1]; Gordon Graff[1]; Jun Liu[1]; [1]Pacific Northwest National Laboratory; [2]Penn State University

Li-ion battery technology is being actively investigated in recent years due to energy and environmental issues. In the past, Li-ion battery is mainly used for portable devices due to its high energy density. However, more research is need in the field of larger scale stationary application which can compliment renewable energy sources like solar or wind power generation. For stationary unlike portable applications, different criteria for Li-ion battery are required since weight and space limitation is less important issue. The more important factor for such application is cost, cycling stability, safety and toxicity. In our work, choice of cathode and anode and its combination in full cell is characterized and presented.

9:30 AM
Synthesis, Orientation and Electrochemical Properties of Nanostructured $LiMPO_4$(M:Fe, Mn, Co) Cathode for Li-Ion Battery: *Daiwon Choi*[1]; Donghai Wang[2]; In-Tae Bae[3]; Zimin Nie[1]; Jie Xiao[1]; Wu Xu[1]; Ji-Guang Zhang[1]; Gary Z. Yang[1]; Gordon Graff[1]; Jun Liu[1]; [1]Pacific Northwest National Laboratory; [2]Penn State University; [3]State University of New York at Binghamton

Demands for batteries with higher energy and power densities are ever-increasing due to the growing energy storage needs for current and future portable electronic devices and electrical vehicles. In this regard, olivine structured $LiMPO_4$ (M: Fe, Mn, Co, Ni) are investigated for alternative cathode materials. However, due to the low intrinsic electronic and ionic conductivity of $LiMPO_4$ (M: Fe, Mn, Co, Ni), it is difficult to utilize the full theoretical capacity at useful rates. Recent studies clearly indicate the critical importance of $LiMPO_4$ (M: Fe, Mn, Co) particle morphology to overcome these limitations. In our study, novel molten surfactant based technique has been developed to obtain nano-sized LiMPO4 (M: Fe, Mn, Co) with improved electrochemical activity. The particle morphology, orientation and electrochemical properties will be presented and discussed.

9:50 AM Break

10:00 AM
GraphiMetal Coatings on High Thermal Conductivity Graphite Foam to Prevent "Dusting" and Facilitate Solder Joining: *Ben Poquette*[1]; Stephen Kampe[2]; [1]Keystone Materials LLC; [2]Michigan Tech

Keystone Materials, LLC utilizes its patent pending GraphiMetalTM coating process to fully metallize graphite foam in a way that does not close the porosity and leaves fluid/air flow though the foams unhindered. The GraphiMetalTM process is readily scalable and does not utilize rare or cost prohibitive materials that could hinder large scale production. The coating method was initially developed at Virginia Tech in conjunction with Oak Ridge National Laboratory (ORNL) to provide solderability for meso-phase pitch derived graphitic foams for the creation of high thermal conductivity joints in heat exchangers. This process facilitates direct joining of coated foams to other metallic structures using traditional soldering techniques. The uniform metal deposit formed also creates a continuous envelope to prevent "dusting" without negatively affecting foam performance. With this improvement, GraphiMetalTM foam has become a viable material to replace traditional metallic thermal materials in energy storage and recovery systems.

10:20 AM
The Effect of Stoichiometry and Sintering Temperature on the Thermoelectric Properties of Titanium Cobaltite: *Biprodas Dutta*[1]; Sezhian Annamalai[1]; Rudra Bhatta[1]; Ian Pegg[1]; [1]The catholic University of America

Calcium cobaltites exhibit superior thermoelectric efficiency among all ceramic materials. While calcium cobaltites have been studied extensively enough attention has not been paid towards other cobaltites. In the present investigation, the thermoelectric properties of titanium cobaltite, which is a paramagnetic material with spinel structure, have been studied. The samples with three different Ti/Co ratios were sintered from 900 to 1250°C. X-ray diffraction and scanning electron microscopy were utilized to perform phase and microstructural analysis to study the evolution of various phases and microstructure as a result of the change in the Ti/Co ratio as well as the sintering temperature. The effect of such changes on resistivity and Seebeck coefficient are also discussed. Resistivity and Seebeck coefficient of $Ti_xCo_{1-x}O_y$ were determined in the temperature range of 300 – 700 K. The activation energies for both electrical conduction as well as thermoelectric transport were calculated and discussed to identify the transport mechanisms.

10:40 AM
Specialized Metal Coatings Unleash the Potential of High Thermal Conductivity Graphite Foam: *Ben Poquette*[1]; Stephen Kampe[2]; [1]Keystone Materials LLC; [2]Michigan Tech

In the late 90's, ORNL developed a technique to fabricate high conductivity graphite foam. With its unique properties, this foam has shown promise to revolutionize the performance of many commercial and defense related systems including: thermal management, inert electrodes and catalyst supports, and acoustic signature management. Until recently, low strength, conductive particle dusting, and difficulties in joining have hindered its incorporation into current platforms. A coating technique was developed at Virginia Tech, which allows a strongly adhered, uniform metallic coating to be applied throughout the thickness of graphite foam. These metal coatings have been shown to solve existing short-falls (low strength, dusting, joinability, etc.) as well as lend their properties (magnetic, catalytic, oxidation resistance, etc.) to graphitic foam without significantly affecting the foam's low density. This lightweight, high conductivity material system should lead to considerable improvements in heat exchanger efficiency for industrial and energy cogeneration systems.

11:00 AM
Development of Advanced Low-Temperature Sodium Beta-Alumina Batteries: Xiaochuan Lu[1]; Guanguang Xia[1]; Kerry Meinhardt[1]; John Lemmon[1]; Vince Sprenkle[1]; Zhenguo Yang[1]; [1]Pacific Northwest National Laboratory

Due to the high round trip efficiency and capability of energy storage for a duration of hours, the sodium ß"-alumina battery technologies have gained increasing interests for renewable and utility applications. The batteries are typically fabricated upon a thick tubular ß"-alumina electrolyte (> 2 mm) with a relatively high operating temperature (> 300ºC) to achieve adequate cell performance. Recently, we attempt to develop battery cells constructed on a thinner planar electrolyte. At the meanwhile, research work has been conducted to modify the cathode both the microstructure and composition in such a way that a satisfactory performance can be achieved at a lower temperature. The details of the work the paper will be presented.

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

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

Thursday AM Room: 211
February 18, 2010 Location: Washington State Convention Center

Session Chairs: Jay Whitacre, Carnegie Mellon Univeristy; Guozhong Cao, University of Washington

8:30 AM
Alternative Catalyst Supports Based on Metal Carbides: *Susanne Opalka*[1]; [1]United Technologies Research Center

Transition metal carbides offer numerous benefits for replacing traditional mesoporous carbon polymer electrolyte membrane fuel cell electrode supports, including good corrosion-resistance and low contact resistance with loaded noble metal catalysts. The oxygen reduction reaction activity and active surface area stability of Pt electrocatalysts loaded on carbide supports, like tungsten carbide, are enhanced by strong electronic Pt-carbide interfacial interactions. The design of strong metal support interactions (SMSI) provides another route to tune catalyst activity, in addition to more traditional approaches of modifying catalyst composition, morphology, and distribution. These SMSI phenomena may result from shifts of: catalyst electron distribution from support electronic donation/withdrawal, electron energy density due to the covalent overlap of support and catalyst electronic orbitals, and energy level broadening from support-catalyst geometric or coordinative interactions. In these regards, atomic modeling will be presented to provide insights into the electronic basis for SMSI phenomena in tungsten carbide supported Pt catalysts.

8:50 AM
Nanoscale Tantalum Oxide Based Catalysts for PEM Fuel Cell Applications: *Jin Kim*[1]; Tak-Keun Oh[1]; Yongsoon Shin[1]; K. Scott Weil[1]; [1]Pacific Northwest National Laboratory

One of key barriers in the commercialization of PEM fuel cells is the use of expensive platinum-based catalysts. Even though a lot of efforts have been made to minimize or eliminate platinum in the electrodes of PEMFCs, none of alternative catalysts show satisfactory properties in term catalytic activity and stability. Based on the unique properties of tantalum oxide such as high oxygen reduction onset potential and excellent stability, we developed nanoscale tantalum oxide/carbon composite catalysts for PEMFC cathode. Nanoscale tantalum oxide/carbon composite catalysts exhibited the improvement in catalytic performance compared to commercial tantalum oxide due to increasing triple-phase boundaries where the oxygen reduction reaction occurs. In this study, the electrochemical performance of nanoscale tantalum oxide based catalysts and the effect of dopants on the electrochemical performance of tantalum oxide have been investigated. The detailed results to date will be discussed.

9:10 AM Invited
Lithium Ion Batteries: Materials Processing and Mechanical Degradation: *Claus Daniel*[1]; Kevin Rhodes[2]; [1]Oak Ridge National Laboratory and University of Tennessee; [2]University of Tennessee

Lithium ion battery technology is projected to be the leapfrog technology for the electrification of the drivetrain and to provide stationary storage solutions to enable the effective use of renewable energy sources. Extensive research and development has enhanced the technology to a stage where it seems very likely that safe and reliable lithium ion batteries will soon be on board hybrid electric and electric vehicles and connected to solar cells and windmills. However, safety of the technology is still a concern, service life is not yet sufficient, and costs are too high. New materials processing technology is needed to reduce cost. Mechanical degradation and fatigue behavior has to be better understood in order to provide microstructural solutions to new and advanced energy storage systems. This presentation will give an overview for a materials science community to bundle forces and help solve our energy problem.

9:50 AM
Low Cost Aqueous Electrolyte Based Energy Storage: Materials and Performance: *Jay Whitacre*[1]; Sangeun Chun[1]; Sanjeev Sharma[1]; Amul Tevar[1]; Andrew Polonsky[1]; [1]Carnegie Mellon Univeristy

Cost is the single largest barrier to wide adoption of energy storage technology for high capacity applications. To this end, we have investigated the possibility of processing ubiquitous and inexpensive precursors to make functional electrode materials for electrochemical energy storage. Anode materials include various high surface are carbons and some Si and Ti based oxides, while cathode materials are transition metal oxides. Since the organic electrolytes used in Li-ion systems are expensive (in part due to the requirement for a dry handling environment), we turn to the higher ionic conductivity aqueous electrolyte systems. The talk will explore different electrode options, the performance of some promising devices in different conditions, and likely future development paths.

10:10 AM Break

10:20 AM Invited
Sol-Gel Derived Lithium Iron Phosphate Films for Efficient Lithium-Ion Intercalation: Yanyi Liu[1]; Dawei Liu[1]; Qifeng Zhang[1]; Betzaida Garcia[1]; *Guozhong Cao*[1]; [1]University of Washington

In this presentation, we will use sol-gel derived nanostructured LiFePO4 thin films as an example to demonstrate the significant influences of the micro-, nano-, and crystal structures on lithium ion intercalation properties. In addition, we will also show the impacts of the surface chemistry, impurity or defects on the phase transition and mass and charge transport accompanied to the lithium ion intercalation-extraction processes. With appropriate control of micro-, nano- and crystal structures and surface chemistry, both high specific energy and specific power are readily achieved. For example, at a current density of 100mA/g, LiFePO4 films demonstrated a lithium-ion intercalation capacity of 250 mAh/g, far exceeding the theoretical storage capacity of conventional LiFePO4 electrode. The presentation will demonstrate the experimental evidences and articulate the relationship between the processing condition, controlled impurity and defects, micro-, nano-, and crystal structures, and the lithium-ion intercalation properties.

11:00 AM
A New Material, Li2Mn2(MoO4)3 for Li-Ion Batteries: Synthesis and Characterization: *K.M. Begam*[1]; S.R.S. Prabaharan[2]; M.S. Michael[3]; [1]Universiti Teknologi PETRONAS; [2]University of Nottingham; [3]SSN Engineering College

The demand for electrically operated devices has led to a variety of energy storage systems amongst which Li-ion batteries substantially impact the areas of energy storage and advanced vehicles. A new polyanion material, Li2Mn2(MoO4)3 is introduced for use as positive electrode in Li-ion batteries. The new material was prepared following a solution based low temperature protocol and found to crystallize in a single phase structure with high phase purity upon annealing the as-prepared product. Rectangular rod-shaped particles having submicrometre dimension were evident from SEM analysis. As for the electrochemical properties, potentiostatic and glavanostatic cycling tests were conducted. The new material was found to exhibit redox peaks corresponding to the transition metals Mn and Mo indicating the electrochemical reversibility as evidenced from Slow Scan Cyclic Voltammetry (SSCV) studies. The charge-discharge profiles obtained by means of Galvanostatic cycling tests signified removal/reinsertion of lithium in the new materials. Key Words: Polyanions, Lithium batteries

11:20 AM
Effect of Co Substitution on the Structural and Electrochemical Behavior of Spinel LiMn2O4: *Rahul Singhal*[1]; Naba Karan[1]; Rajesh Katiyar[1]; Ram Katiyar[1]; [1]University of Puerto Rico

We have synthesized LiMn2-xCoxO4 (x = 0, 0.03, 0.05, 0.10, 0.25, and 0.50) cathode materials by sol-gel method. The phase pure materials were obtained at an annealing temperature of 875oC for 15 h. The materials were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive analysis by X-ray (EDAX), and micro Raman spectroscopy. The cathodes and coin cells were prepared as reported earlier1. The electrochemical behavior of the cathode materials were studied using cyclic voltammetry and charge-discharge characteristics. LiMn1.97Co0.03O4 cathode material showed an initial discharge capacity of 133.72 mAh/g, with 89% capacity retention, after 50 charge-discharge cycles. It was found that as the cobalt concentration increases, the discharge capacity decreases gradually. The detailed structural and electrochemical results will be presented during the meeting. References: 1. R. Singhal, M.S. Tomar, S.R. Das, S.P. Singh, A. Kumar, R.S. Katiyar, Electrochemical and Solid-State Letters, 10(7) 2007, A163.

11:40 AM
Mg_3N_2-Li-Mg Cermet Anodes for Lithium Based Batteries: *Alpesh Khushalchand Shukla*[1]; Thomas Richardson[1]; [1]Lawrence Berkeley National Laboratory

Lithium alloys have been considered as attractive candidates to replace graphite in anodes for lithium based batteries, mainly due to their high theoretical capacities. However, these alloys suffer from significant irreversible capacities, poor cyclability and rate capability. In this study, Lithium rich ceramic-metal composites, or cermets, were developed using a simple metathesis reaction were developed and characterized using transmission electron microscopy and electron energy loss spectroscopy. The cermets were prepared by mixing Li_3N powder with Mg powder and heating them to the melting temperature of the alloy phase. This resulted in a composite which consisted of Mg_3N_2 particles embedded in a Li or Li-Mg matrix. Cycling experiments were also carried out, and preliminary results showed that the Li-Mg cermets performed better thatn their alloy counterparts in terms of rate capability and potential relaxation following stripping.

Modeling, Simulation, and Theory of Nanomechanical Materials Behavior: Nanoindentation and Contact Mechanics

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

Thursday AM — Room: 304
February 18, 2010 — Location: Washington State Convention Center

Session Chairs: Dylan Morris, NIST; Lawrence Friedman, NIST

8:30 AM Invited
Plastic Deformation of Au Particles on a Sapphire Substrate: Dan Mordehai[1]; Eugen Rabkin[1]; *David Srolovitz*[2]; [1]Technion - Israel Institute of Technology; [2]Yeshiva University

We report a combined experimental/molecular dynamics study of the indentation of faceted Au nanoparticles on a sapphire surface. The particles were created via the agglomeration of a polycrystalline Au film. Indentations were also performed in Au films of similar dimensions. Both simulations and experiment show that the particles are softer than the film and that the deformation behavior is nearly independent of particle size. Deformation is controlled by dislocation nucleation near the indentor, followed by fast dislocation glide toward the surface. Well defined pile-ups were observed near the indents in thin films, while no such pile-ups were observed in the particles. We present a comparison of post-deformation particle shapes from high resolution AFM and thesimulations.

9:00 AM
Effect of Temperature on Nano-scale Asperity Contact and Separation in Au: *Jun Song*[1]; David Srolovitz[2]; [1]Brown University; [2]Yeshiva University

We performed a series of molecular dynamics simulations of contact and separation of two Au surfaces at different temperatures; one with a single, initially hemispherical asperity and the other flat. We monitor the force between the two surfaces and the symmetry order parameter together with the atomic structure during loading and unloading at each temperature. The pull-off force decreases monotonically with increasing temperature except for an abrupt rise that occurs between T1=T=T2. This abrupt rise can be traced to a series of phase transformation in the sample during separation (FCC->HCP->FCC) at elevated temperatures. The FCC->HCP->FCC process transforms the system from the original FCC structure to one that is in a twin orientation relative to the original FCC structure. The new FCC structure has a lower Schmid factor than the original FCC structure and consequently exhibits higher tensile strength.

9:20 AM
The Strongest Contact and Size Effect in Nanoscale Metal-Metal Contact: Molecular Dynamics Simulation Study: *Hojin Kim*[1]; Alejandro Strachan[1]; [1]Purdue University

We characterize the tensile strength of the nanoscale contacts formed when two clean platinum asperities are brought together by using large-scale molecular dynamics simulation. Simulation results show that the tensile strength of the nanoscale contacts exhibits significant size effect with a maximum at approximately 5 nm contact size. As we know, it is the first time to appear a "strongest size" in single crystals. This size effect connects with the density of dislocations that are generated during contact closing and opening. A reduction of initial dislocation density (created during contact closing) and an increasing difficulty in the production of dislocations during contact opening cause to weaken strength as size decrease down to 5 nm. The strongest contact occurs when the density of dislocations during closing becomes a minimum and the following strength decrease with decreasing size is due to reduced constraints to mechanical deformation by the slabs.

9:40 AM Invited
Friction and Adhesion at the Nanoscale: *Izabela Szlufarska*[1]; Yifei Mo[1]; Yun Liu[1]; [1]Universty of Wisconsin

Friction and adhesion are particularly important for mechanical performance of nanoscale devices, where surface-to-volume ratio is high. Two major challenges to understanding nanoscale friction are: (i) Macroscopic laws do not apply to nanoscale contacts; (ii) It is not possible to predict friction force because of the complexity of energy dissipation mechanisms involved in sliding (e.g., dislocations, phonons, surface chemistry). This talk will focus on fundamental understanding of nanoscale tribology gained through molecular dynamics (MD) and ab initio methods. MD simulations have been used to determine friction laws in dry nanoscale contacts. Two specific contributions to friction will be discussed: adhesion and adsorbate atoms. Using Si and SiC as model systems, it is shown that adhesion can be controlled by surface strain and chemistry. Hydrogen and deuterium adsorbates on diamond are used to explore dependence of friction on vibrational excitations and on surface coverage.

10:10 AM Break

10:30 AM Invited
Dislocation Nucleation, Jerky Flow and Size Effects in Nanoindentation: Wei Wang[1]; Yuan Zhong[2]; Garritt Tucker[2]; Ke Lu[1]; Lei Lu[1]; *David McDowell*[2]; Ting Zhu[2]; [1]Shenyang National Laboratory for Materials Science; [2]Georgia Institute of Technology

Recent results from MD simulations regarding homogeneous and heterogeneous dislocation nucleation in fcc crystals are summarized, with emphasis on non-Schmid effects and reordering processes. It is shown that the activation volume for homogeneous nucleation is on the order of a few b3 at high stress levels characteristic of nanoindentation. Deeper insight into stochastic jerky plastic flow during nanoindentation of single crystal copper is gained by combining experiments, statistical analyses, and atomistic simulations. The nanoindentation size effect on yield strength arises in concert with extreme value statistics of dislocation sources. Source activation induces a dislocation avalanche and indenter displacement burst, and its probability decreases with the radius of the indenter tip. Our results demonstrate that jerky plastic flow can be caused by the activation of either surface or bulk dislocation sources, with sensitivity to the orientation of the crystal relative to the indentation direction.

11:00 AM
Assessment of the Hertzian Estimate of Plasticity-Initiating Shear Stresses during Nanoindentation: *Dylan Morris*[1]; Li Ma[1]; Lyle Levine[1]; Stefhanni Jennerjohn[2]; David Bahr[2]; [1]NIST; [2]Washington State University

The sudden onset of plasticity during nanoindentation of metals is associated with dislocation nucleation, multiplication, and propagation. The shear stresses responsible for the sudden onset of plasticity are typically estimated from Hertzian contact mechanics. Here, a critical assessment of possible errors and pitfalls in the experimental measurement of plastic-onset stresses is made. The near-apex shape of Berkovich probes – one sharp, and one worn – was measured by scanning probe microscopy. These data were used as "virtual" indentation probes in a 3-dimensional finite-element analysis (FEA) of indentation on <100>-oriented single-crystal tungsten. Experiments were also carried out with those probes on <100>-oriented tungsten. Excellent agreement is found between experimental and FEA force-displacement relationships, but the discrepancies between Hertzian and FEA estimates of the controlling shear stresses are larger than 30%.

11:20 AM
Atomic-Scale Study of Nanoindentation in Iron and Copper: *Yury Osetskiy*[1]; Chansun Shin[2]; Roger Stoller[1]; [1]ORNL; [2]Korea Atomic Energy Research Institute

We present results of extensive molecular dynamics study of materials deformation during nanoindentation process in Fe and Cu. We have used different indentation surfaces namely ½{110} and {100} in Fe and ½{111} and {100} in Cu and spherical rigid indenters of diameter from 5 to 40 nm at indentation speeds of 2 m/s and 10 m/s in crystals of up to 1.1x108 atoms. Plastic deformation at early stages or by small size indenter occurred mainly by emission of glissile dislocation loops. Large indenters may create complex three-dimensional structures that affect strongly the deformation process. Dislocation junctions of different structures and mobility were observed and classified from the point of view of their effects to nanoindentation process. A higher indentation loading rate was observed to promote the formation of shear loops on a nucleated circular dislocation in Fe.

11:40 AM
Nanoindentation Simulations to Predict Macroscale Properties of Cement: *Priscilla Fonseca*[1]; [1]Northwestern University

The microstructure of cementitious materials determines most of their macroscale properties, such as strength, permeability, shrinkage, and creep. As new types of cement are developed, it becomes important to develop predictive models that connect the microstructure to macroscale behavior. Calcium silicate hydrate (C-S-H), the primary binding phase of concrete, is responsible for macroscale cohesion and durability. This talk presents a numerical model of the nanostructure of C-S-H and its capability to predict macroscale properties. Generated using an autocatalytic growth algorithm, C-S-H as an assemblage of discrete granular particles will be introduced with particle-scale properties such as elastic modulus, friction, and surface charge. Using DEM simulations, macroscale indentation properties of hardened cement paste are quantitatively predicted. This predictive capability suggests that it is possible to numerically determine macroscale properties relating to the durability of concrete for new cement mix designs without engaging in extensive experimental testing.

Neutron and X-Ray Studies of Advanced Materials III: Diffraction Analysis of Alloys

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

Thursday AM Room: 303
February 18, 2010 Location: Washington State Convention Center

Session Chairs: Jaimie Tiley, Air Force Research Laboratory; Erica Lilleodden, GKSS Research Center

8:30 AM Keynote
Simulating Realistic Conditions and In-Situ Studies Using Neutron Diffraction: *Ron Rogge*[1]; [1]National Research Council

The high penetration of neutrons in most industrial materials permits examining the material's response to external influences throughout its volume. The high penetration also enables relatively straightforward development of sample environments. These can be used for fundamental studies of material response in order to understand the material or guide development of new materials. Other environments may simulate manufacturing conditions in order to evaluate or improve processes and others simulate in-service conditions, which can contribute to fitness-for-service evaluations. A variety of examples will be presented demonstrating each of these.

9:00 AM
Why Neutrons to Study Superalloys?: *Ralph Gilles*[1]; Pavel Strunz[2]; Debashis Mukherji[3]; [1]TU Muenchen; [2]Nuclear Physics Institute; [3]TU Braunschweig

Characterization of microstructure in superalloys is predominantly carried out with microscopic methods. Due to the low penetration of X-rays, electrons or light the samples have to be very thin by using transmission methods or the investigation is limited to the surface. Neutrons enable to enlarge the investigated sample volume, both the cross section due to the large size of neutron beams and the thickness up to a few millimeters thanks to the favorable penetration depth. In superalloys, for example in situ measurements at high temperatures are quite often useful. The detection of detrimental phases like TCP phases, or the determination of lattice misfit between precipitate and matrix, demonstrated how worthwhile it is using the non-destructive tools of small-angle neutron scattering and neutron diffraction. Examples will be discussed to show the advantages and the complementary of neutrons to X-ray and electron radiation. Reference: R. Gilles, Z. Metallkd. 96 (2005), 4, 325-334.

9:15 AM
Determining the Impact of Cooling Rate and Aging Times on Nickel Base Super Alloys Using Callibrated XRD Intensity Ratioswhich Courses Were Actually Held?: *Jaimie Tiley*[1]; R Banerjee[2]; [1]AFRL/RXLMD; [2]University of Texas

Determining the volume fraction of gamma prime phases within nickel base superalloys is difficult due to nanometer sized tertiary gamma prime precipitates. This research develops callibration curves based on ordered intensity peaks for different volume fractions of Rene88 gamma prime and gamma powders extracted from bulk material samples. The curves are used to determine volume fractions of bulk samples using synchrotron data. Volume fractions and misfit strains are obtained for water quenched and slow cooled samples aged up to 200 hours at 760°C.

9:30 AM Invited
Deformation Of Shape Memory Alloys Under Biaxial Loading: *Donald Brown*[1]; Catherine Tupper[2]; Vaidyanathan Raj[3]; Deniece Korzekwa[1]; Sisneros Thomas[1]; Clausen Bjorn`[1]; [1]Los Alamos National Lab; [2]Northwestern University; [3]University of Central Florida

We have made a concerted effort on SMARTS to study shape memory alloys (SMA's) under their operating conditions. This has included the development of sample environments to allow straining measurements at high and low temperatures, in magnetic fields, and under cyclic deformation. Most recently, we have developed the capability to study SMA's under biaxial tensile deformation.

Both UNb and NiTi have been studied in-situ during uniaxial deformation using neutron diffraction techniques. However, applications seldom require uniaxial deformation of SMA's, but rather require more complicated deformation paths. Using hydraulic bulge test and in-situ neutron diffraction experiments, we have examined the strain and texture evolution in both shape memory systems in-situ under biaxial loading conditions. Equivalent through-thickness and membrane strains are compared to both tensile and compressive uniaxial measurements in order to evaluate the deformation mechanisms under the disparate loading conditions.

9:50 AM
In-Situ Observation of Strain Evolution in CP-Ti over Multiple Length Scales: *Colleen Bettles*[1]; Peter Lynch[2]; Andrew Stevenson[2]; Dacian Tomus[1]; Mark Gibson[2]; Kia Wallwark[3]; Justin Kimpton[3]; [1]ARC Centre of Excellence for Design in Light Metals, Monash University; [2]CSIRO Materials Science and Engineering; [3]Australian Synchrotron

The strain evolution in polycrystalline CP-Ti strip under tension was studied, in-situ and at two length scales, using Synchrotron X-ray diffraction. To establish the bulk material behaviour, experiments were performed at the Australian synchrotron facility. Owing to the relatively large grain size, discontinuous 'spotty' Debye ring patterns were observed, and a peak fitting algorithm was developed to determine the individual spot positions with the necessary precision for strain determination. The crystallographic directional dependence of strain anisotropy during the loading cycle was determined. Strain anisotropy and yielding of individual crystallographic planes prior to the macroscopic yield point were further clarified by in-situ loading experiments performed at the Advanced Light Source. The deviatoric strain accumulation and plastic response were mapped on a grain by grain basis. The onset of microscopic yielding in the grains was identified and correlated with the relative orientation of the grains with respect to the loading direction.

10:05 AM
Influence of Strain Rate on Mechanical Properties and Crystallographic Texture of Hot-Pressed and Rolled Beryllium: *Thomas Sisneros*[1]; Donald Brown[1]; Bjorn Clausen[1]; Saurabh Kabra[1]; William Blumenthal[1]; [1]Los Alamos National Lab

Plastic deformation of hexagonal metals such as beryllium occurs by a mix of slip and twinning mechanisms. Deformation slip and twinning are controlled by different mechanisms at the atomic scale, and thus respond differently to variations in strain rate. In general, deformation twinning is expected to be favored by high strain rate conditions. Strongly textured and random beryllium samples were deformed at strain rates from 0.0001/sec to 5000/sec. The yield point is strain rate insensitive over 7+ orders of magnitude of strain rate. The hardening, however, is strongly rate dependent. Optical microscopy and neutron diffraction measurement of crystallographic texture were carried out to monitor the evolution of the microstructure and specifically the activity of mechanical twinning as a function of strain rate. The relative roles of the active slip and twin deformation mechanisms are linked to the observed rate dependence of the flow stress.

10:15 AM
In-situ Neutron-Diffraction and Thermal Characterization of Fatigue Behavior: *E-Wen Huang*[1]; Rozaliya Barabash[2]; Bjørn Clausen[3]; Yee-Lang Liu[4]; Ji-Jung Kai[4]; Wenjun Liu[5]; Gene Ice[2]; Peter Liaw[1]; [1]University of Tennessee; [2]Oak Ridge National Laboratory; [3]Los Alamos National Laboratory; [4]National Tsing-Hua University; [5]Argonne National Laboratory

Cyclic loading and the subsequent temperature evolution of the lattice strain have been investigated with in-situ neutron-diffraction and thermal characterization for a nickel-base alloy. The lattice strain and thermal response to the applied load are investigated as a function of the fatigue cycles. Fatigue damage is observed with bulk hardening, softening, and eventual saturation evident in the diffraction patterns and the thermal-evolution features. An increase in dislocation density is responsible for hardening during the first cycles. The transition to saturation cycles is characterized by the anisotropy of the lattice-strain evolution. Moreover, inhomogeneity of the thermal response and irreversible compression of the lattice planes are observed in the final saturation fatigue cycles. The local fatigue damages are quantitatively studied by the polychromatic X-ray microdiffraction and transmission electron microscopy. The ex-situ results are discussed along with the in-situ measurements. The development of irreversible microstructure are discussed.

10:25 AM
In-situ Neutron Diffraction Experiments as a Guide for Understanding the Microstructure Evolution during Deformation of Complex Materials: *Steven Van Petegem*[1]; Alexander Evans[1]; Helena Van Swygenhoven[1]; [1]Paul Scherrer Institut

Predicting the development of intra- and intergranular stresses during deformation is a challenging task, especially for materials with a complex microstructure such as advanced steels and multiphase engineering components. A detailed knowledge of these so-called 'microstresses' is of utmost importance for understanding the influence of microstructure exerted on the mechanical properties. Here we present some recent results obtained at POLDI, the Time-Of-Flight diffractometer at SINQ (Paul Scherrer Institut). In particular we focus on the development of microstresses during uni-axial tensile deformation of some multiphase advanced steels. We report on the complex interplay between elastic and plastic anisotropy, which is responsible for the built-up of large residual stresses. Furthermore we demonstrate how in-situ x-ray diffraction can be used as a complementary tool to reveal the role of those phases which are invisible for neutrons because of their low volume fraction and/or chemical nature.

10:40 AM
Real Time Synchrotron Radiography of High Temperature High Cycle Fatigue Crack Growth in Single-Crystal Nickel-Base Superalloys: *Clinique Brundidge*[1]; Naji Husseini[1]; Erik Hanson[1]; Chris Torbet[1]; Roy Clarke[1]; J. Wayne Jones[1]; Tresa Pollock[1]; [1]University of Michigan

High temperature ultrasonic fatigue experiments were performed at the Advanced Photon Source at Argonne National Laboratory in order to image, in situ, the fatigue crack growth (FCG) in a single-crystal nickel-base superalloy using high brilliance x-ray undulator radiation. A portable ultrasonic fatigue instrument was used to produce a frequency of 20 kHz (R=0.1) with axial loading in the <001> direction. A micro-torch heated samples between 538°C to 982°C. Fatigue cracks emanating from notched samples with a 200µm thickness were observed (through-thickness) with x-ray radiographs taken every thousand cycles over tens of millions of cycles showing micron-by-micron crack growth. Crystallographic cracks propagated along specific planes at temperatures below 760°C and non-crystallographic crack growth became more prevalent as the temperature increased. For well-oriented samples, cracks propagated along {111} slip planes, however, misoriented samples produced crack growth on alternative planes. The influence of cast microstructural features and temperature on FCG will be discussed.

10:50 AM
Evolution of Crystallographic Texture of TRIP Steel under Forming Load Conditions: *Adam Creuziger*[1]; Thomas Gnaeupel-Herold[1]; Tim Foecke[1]; [1]National Institute of Standards and Technology

TRIP (Transformation Induced Plasticity) steels are a relatively new multi-phase, high strength, high ductility steel alloy being investigated by the automotive industry to improve fuel economy. In this study, as received TRIP steel sheets are deformed under uniaxial, plane strain and balanced biaxial strain conditions. After deformation the micro-structural properties of the deformed material are investigated using neutron diffraction to determine the phase fractions in the deformed material and how the crystallographic texture evolves as a function of strain for each deformation mode. Using crystallographic theory of martensite (CTM), theoretical predictions for the austenite transformation as a function of texture and stress state are compared to the measured texture.

11:05 AM Break

11:15 AM
Software Tools for the Monitoring, Analysis and Interpretation of Engineering Neutron Diffraction Data: Seung Yub Lee[1]; Youngshin Kim[1]; Hyuntae Na[1]; *Ersan Ustundag*[1]; [1]Iowa State University

Proper analysis and interpretation of engineering neutron diffraction (ND) data requires the solution of an inverse problem where experimental data are compared to the predictions of crystallographic and materials models. This process involves numerous parameters, some of which may be highly correlated, and without proper software tools can be rather difficult to handle. As part of the DANSE project (danse.us), we have been developing tools that will not only aid the user in this process, but will also allow real-time monitoring and analysis of data for a more efficient use of beam time. This presentation will also describe tools that perform full experiment simulation. Our ultimate goal is to help establish ND data analysis and interpretation on a more rigorous theoretical and computational foundation.

11:30 AM

Transformation Pathways in High Temperature Shape Memory Alloy Candidates Based on the NiTi, NiMnGa and ZrCu Alloy Systems: *Mohammed Azeem*[1]; Seema Raghunathan[1]; David Dye[1]; [1]Imperial College

High temperature (>200 °C) shape memory alloys (HTSMAs) would be of great interest, e.g. in aerospace applications. Here, synchrotron X-ray diffraction is used to characterise the evolution of phase assemblage and texture during thermal cycling of several candidate HTSMA systems - NiTi, NiMnGa and ZrCu, in polycrystalline rolled strip. It is shown that Af transformation temperatures in excess of 200°C can readily be achieved but that Mf temperatures in excess of this are harder to achieve. Temperature hysteresis is typically greater than that observed in NiTi. Cyclic stability is also problematic, although there are well-known approaches to mitigate this problem. In Ni54Mn25Ga21 a two-step transformation is observed, while in Ni50Ti35Hf7.5Zr7.5 martensite can be retained on cycling. It is also noted that DSC experimentation alone is a poor guide to behaviour, as it is insensitive to the transformation pathways of the alloys.

11:45 AM

Martensitic Transformation Induced Plasticity in Nanostructured Steel: A High-Energy X-Ray Diffraction Study: *Sheng Cheng*[1]; Hahn Choo[1]; Yandong Wang[2]; Xun-Li Wang[3]; Jon Almer[4]; Peter Liaw[1]; Young-Kook Lee[5]; [1]University of Tennessee; [2]Northeast University of China; [3]Oak Ridge National Laboratory; [4]Argonne National Laboratory; [5]Yonsei University

In contrast to the poor tensile behavior in most nanostructured materials, a recently-developed metastable austenite steel was demonstrated with high strength and outstanding tensile ductility, owing to the contribution from transformation-induced plasticity (TRIP) effect. To understand the contribution of the martensitic transformation, an in situ synchrotron X-ray diffraction was conducted. With the analysis of load-partitioning behavior, transformation kinetics, as well as the texture evolution, it is revealed that the martensitic transformation contributed greatly to the plastic deformation in first stage of deformation, while the dislocation-based mechanism mainly contributed to the second stage. Different from the coarse-grained sample, the martensitic transformation was mainly propelled through Lüders band propagation, which was elaborately explored by micro-beam scanning. This work was supported by the National Science Foundation Major Research Instrumentation (MRI) Program (DMR-0421219) and International Materials Institutes (IMI).

12:00 PM

Mechanical Behavior and Microstructure Evolutions in a Nanocrystalline Ni-Fe Alloy: *Li Li*[1]; Tamas Ungar[2]; Yandong Wang[3]; Yang Ren[4]; Hahn Choo[1]; Peter Liaw[1]; [1]Department of Materials Science and Engineering, The University of Tennessee; [2]Department of Materials Physics, Eötvös University; [3]School of Materials Science and Engineering, Beijing Institute of Technology; [4]X-Ray Science Division, Argonne National Laboratory

Bulk nanocrystalline Ni-Fe alloy with grain size around 20 nm is rolled to 10%, 20%, and 30% reductions at both room temperature and liquid-nitrogen temperature, respectively. Hardness tests are performed in the prepared samples. Synchrotron high-energy X-ray diffraction and X-ray line profile analysis are applied in the experiments and in data reductions. The microstructure evolutions such as dislocation density, grain size, and twin density are investigated in the above mentioned samples. Temperature effects and deformation level are considered in the deformation study. This study will provide detailed microstructure information for explaining the exhibited mechanical behaviors and unveiling the underlying deformation mechanisms in bulk nanocrystalline Ni-Fe alloy.

12:10 PM

Neutron Diffraction Study of the Internal Stress and Strain States of a Single Crystal Superalloy under Different Heat Treatment Conditions: *Erdong Wu*[1]; Guangai Sun[2]; Bo Chen[2]; Sucheng Wang[1]; Thilo Pirling[3]; Darren Hughes[3]; [1]Institute of Metal Research, Chinese Academy of Science; [2]Institute of Nuclear Physics and Chemistry; [3]Institut Laue Langevin

The microstructures of the nickel-based single crystal superalloy vary considerably under different heat-treatment conditions, which strongly affect the high temperature mechanical properties of the superalloy. A neutron diffraction investigation of the lattice mismatches of the γ-matrix and the γ'-precipitate phases of a superalloy involving thorough examinations of the superlattice of the γ'-precipitates demonstrates that the relevant diffraction contours are strongly indices dependent, and differ significantly for different phases and different microstructures. These contour variations are analyzed to characterize the internal stress and strain states, and associates the microstructures to the high temperature mechanical properties of the superalloy. The correlations between the interphase stress and the intraphase strain induced by the evolution of the γ'-precipitates from the γ-matrix and the relevant lattice-mismatch changes during different heat treatments of the superalloy are revealed and discussed based on the calculation and relevant dislocation modeling of the internal stress and strain states.

12:25 PM

Understanding the Texture Development during Biaxial Mechanical Loading: *Ercan Cakmak*[1]; Hahn Choo[1]; [1]Department of Materials Science and Engineering, The University of Tennessee

Fundamental understanding of the evolution of microstructure(intergranular strain, texture, etc.) during biaxial mechanical loading is of significant scientific and technical importance because torsional loading or the combination of torsion and tension/compression loading conditions better represent the realistic manufacturing conditions of most engineering materials compared to simpler uniaxial loading conditions. In this study, texture development during biaxial loading of a model fcc polycrystal is investigated by performing systematic measurements as a function of: (1) loading path (pure torsion with free ends, pure torsion with fixed ends, torsion/tension, torsion/compression as well as pure tension and compression as baseline measurements), (2) applied (shear and normal) strain, and (3) position along the radial direction of the specimen. The experimental results provide a clear understanding of the evolution of texture during biaxial loading by allowing us to deconvolute the various effects of different loading paths on the observed texture components and their interactions.

12:35 PM

High Pressure Deformation of Zirconium: *James Wilkerson*[1]; David Weldon[1]; Sven Vogel[1]; Donald Brown[1]; Carlos Tomé[1]; Sébastien Merkel[2]; [1]Los Alamos National Laboratory; [2]Laboratoire de Structure et Propriétés de l'Etat Solide Université de Lille

Uni-axial deformation of pure Zirconium was performed with the D-DIA apparatus at the APS. The transformation from α-Zr to ω-Zr was observed at ~4.5 GPa at room temperature with the applied pressure derived from the unit cell volume of α-Zr and the known equation of state. A combination of texture analysis of the diffraction data and texture modeling allows to establish the orientation relationship between the two phases for the first time with a large number of grains. After the transformation, the D-DIA apparatus allows to deform the ω-Zr and study deformation mechanism such as slip and twinning activities. We will present first results of this study and compare the deformation modes at ~5 and 8~GPa.

12:50 PM

Modelling and Characterisation of Gamma Prime (γ') Evolution in a Nickel-Base Superalloy Using Small-Angle Neutron Scattering: *David Collins*[1]; Richard Heenan[2]; Howard Stone[1]; [1]University of Cambridge; [2]ISIS Facility, Rutherford Appleton Laboratory

Small angle neutron scattering (SANS) has been used to evaluate the temporal evolution of γ' precipitates in the nickel-base superalloy, RR1000, in situ during a 16 hour heat treatment at 760°C following a supersolvus heat treatment and oil quench. The bimodal distribution of secondary and tertiary γ' was analysed using a specially developed polydispersive model capable of evaluating the scattering curves to obtain precipitate size distributions and volume fractions as a function of time. The results show an increase in volume fraction of secondary γ' at the expense of tertiary γ', as may be expected from Ostwald ripening, along with the simultaneous coarsening of both distributions. The model was designed to be suitable for high volume fractions of γ', and for the scattering interaction between precipitates. The initial and final precipitate distributions have been characterised using TEM, and show satisfactory correlation with the SANS data across the scattering vector range.

Nuclear Energy: Processes and Policies: Material Development

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

Thursday AM Room: 201
February 18, 2010 Location: Washington State Convention Center

Session Chairs: Sue Lesica, US Department of Energy; Mark Bourke, Los Alamos National Laboratory

8:30 AM Keynote
Core Materials Development for Fast Reactors: *Stuart Maloy*[1]; M. Toloczko[2]; J. Cole[3]; Byun[4]; [1]Los Alamos National Laboratory; [2]Pacific Northwest National Laboratory; [3]Idaho National Laboratory; [4]Oak Ridge National Laboratory

The Advanced Fuel Cycle Initiative is investigating methods of burning minor actinides in a transmutation fuel. To achieve this goal, the fast reactor core materials (cladding and duct) must be able to withstand very high doses (>300 dpa design goal) while in contact with the coolant and the fuel. Thus, these materials must withstand radiation effects that promote low temperature embrittlement, high temperature helium embrittlement, swelling, accelerated creep, corrosion with the coolant, and chemical interaction with the fuel (FCCI). Research is underway that includes determining radiation effects in ferritic/martensitic steels at doses up to 200 dpa, testing and development of liners and coatings to prevent/reduce FCCI, and developing advanced alloys with improved irradiation resistance. A summary and status of these studies will be presented with plans for future research.

9:05 AM
Developments in Powder Production for Nano-Structured Ferritic Alloys: *David Hoelzer*[1]; Jim Bentley[1]; Michael Miller[1]; Brian Wirth[2]; Yong Kim[2]; Matt Ferry[3]; Jean Stewart[3]; [1]Oak Ridge National Laboratory; [2]University of California, Berkeley; [3]Crucible Research

Mechanical alloying is commonly used for producing oxide dispersion strengthened (ODS) alloys, including the 14YWT nanostructured ferritic alloy (NFA) containing nanoclusters (NC), since bulk products can be produced from metals and alloys, especially those that have low oxygen solubility. However, a significant problem that adversely affects the mechanical properties of ODS alloys is non-uniformity of oxide dispersions caused by poor mechanical mixing of the oxide and metal or pre-alloyed powders by ball milling. In this study, pre-alloyed Fe powders containing Y and O additions were produced by Ar atomization. The effectiveness that the modified powders have on the uniformity of NC in 14YWT will be presented.This research was sponsored by the Office of Nuclear Energy, Science and Technology and 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.

9:30 AM
Growth Kinetics and Phase Development in Diffusion Couples: U-Mo vs. Al-Si: *Emmanuel Perez*[1]; Dennis Keiser[2]; Yongho Sohn[1]; [1]University of Central Florida; [2]Idaho National Laboratory

Interdiffusion and microstructural development in U-Mo-Al-Si system was examined using solid-to-solid diffusion couples, U-7wt.%Mo, U-10wt.%Mo and U-12wt.%Mo vs. Al, Al-2wt.%Si, Al-5wt.%Si annealed at 550°C for 1, 5 and 20 hours. Microstructural and compositional analyses were carried out by analytical microscopy and spectroscopy. Results were compiled to elucidate the evolution of the interdiffusion layer that develops between the U-Mo and Al-Si alloys. Alloying Si into Al caused a significant reduction in the thickness of the interdiffusion layer. TEM identified UAl3, UMo2Al20, U6Mo4Al43 and UAl4 phases in the interdiffusion layer for U-Mo vs. Al diffusion couples. When Si was added to the Al, and U-Mo vs. Al-Si diffusion couples were examined, only (U,Mo)(Al,Si)3 and UMo2Al20 phases were identified by TEM. The disappearance of U6Mo4Al43 and UAl4 phases and/or solutioning of UAl3 into (U,Mo)(Al,Si)3 may be responsible for the slower growth of the interdiffusion zones in the U-Mo vs. Al-Si diffusion couples.

9:55 AM
Ion Irradiation of an Ultrafine Grained 316 Austenitic Stainless Steel: *Auriane Etienne*[1]; Bertrand Radiguet[1]; Philippe Pareige[1]; Ruslan Valiev[2]; [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, it's proved that only the combination of all microstructural changes (formation of point defect (PD) clusters, solute clustering, radiation-induced segregation at grain boundaries (GB)…) observed under irradiation can lead to IASCC. Since all these changes are due to PD super-saturation, increasing PD annihilation at sinks, such as GB, could limit IASCC. A 316 ASS was nano-structured by high pressure torsion. To study the effect of irradiation, samples were irradiated with 160keV Fe+ at 350°C. Irradiated samples were studied by transmission electron microscopy to see nano-grain size evolution as well as by atom probe tomography to observe the solute atom distribution evolution. The nanostructure evolution is compared to previous examinations of ion irradiated "large grain" 316 ASS.

10:20 AM Break

10:35 AM
Radiation Response of High Temperature, Ultrafine-Precipitation-Strengthened Steel: *Yong Yang*[1]; Todd Allen[1]; [1]University of Wisconsin-Madison

Fast reactor cladding could be improved by increasing the swelling resistance and high temperature strength of an austenitic steel through the inclusion of a high density of nanometer-sized precipitates such as the High Temperature, Ultrafine-precipitation-strengthened Steel (HT-UPS) developed by Oak Ridge National Laboratory. However, the radiation response of the HT-UPS is not well known. In our study, HT-UPS is irradiated with a 2.0MeV proton beam at 300 and 500ºC for various doses up to 3 dpa. The irradiation hardening is evaluated using micro-Vickers hardness test, and the irradiation microstructures are examined using the transmission electron microscopy. Specifically, the stability of nano-sized precipitates is studied using the carbon extraction replica technique.

11:00 AM
Friction Stir Welding of Dispersion-Strengthened Alloy MA754: *Jiye Wang*[1]; Wei Yuan[1]; Rajiv Mishra[1]; Indrajit Charit[2]; [1]Missouri University of Science and Technology; [2]University of Idaho

Friction stir welding of MA754, an Y2O3 dispersion-strengthened superalloy, were investigated. The research is supported by the DOE through grant # DE-FG07-08ID14925. A tool rotation rate of 1000 rpm and a traverse speed of 50.8 mm per minute were employed with a tungsten carbide tool. Tensile behavior of the nugget was compared with that of parent material at various temperatures. Results indicated that a refinement of grain size during friction stir welding leads to improved ductility without the loss of strength at room temperature.

11:25 AM
Development of a Simplified Powder Processing Method for Production of Oxide Dispersion Strengthened Ferritic Alloys: *Joel Rieken*[1]; I. Anderson[2]; M. Kramer[2]; [1]Iowa State University; [2]Ames Laboratory

A simplified powder processing method was used to form an oxide dispersion strengthened ferritic stainless steel microstructure. Precursor ferritic stainless steel powders were oxidized in situ using a newly developed gas atomization reaction synthesis technique. The as-atomized powders contained an ultra thin kinetically favored (i.e., Cr-enriched) surface oxide. This surface layer was used as a vehicle to carry oxygen into the as-consolidated alloy microstructure, where heat treatments were designed to drive oxygen exchange between the less stable prior particle boundary oxide and dissolved Y and other additions. Exchange reactions and subsequent thermal-mechanical processing resulted in nano-metric Y-enriched oxide dispersoids and ultimate strengthening from dislocation sub-structures. Transmission electron microscopy and synchrotron X-ray diffraction helped evaluate the evolution of the alloy microstructure and elevated temperature tensile testing was used to assess the strength of the alloy. Support from the DOE-FE (ARM program) through Ames Laboratory contract no. DE-AC02-07CH11358 is gratefully acknowledged.

11:50 AM
Impact of Zirconium Hydride Precipitates on Fracture of Zirconium Alloys: *Matthew Kerr*[1]; Mark Daymond[2]; Richard Holt[2]; Jonathan Almer[3]; Stephanie Stafford[4]; [1]US Nuclear Regulatory Commission; [2]Queen's University; [3]Argonne National Lab; [4]Kinectrics Inc

Zirconium alloys are of major importance to the nuclear industry, with primary application as a structural material for the in-reactor environment. The formation of brittle hydrides within zirconium alloys results in a degradation of the mechanical properties of the component in which they form. Thus, the rate and characteristics of formation as well as the subsequent impact of these hydrides are critical factors in the determination of zirconium component service life. We have carried out a three part study of hydrides in zirconium using high energy synchrotron x-ray diffraction. Part I characterized the mechanical response of zirconium hydride, in situ within a bulk Zircaloy-2 matrix. Part II studied the near crack tip behavior of un-hydrided Zircaloy-2. Part III characterizes the effect of notch tip hydrides; the aim is to quantify the influence of hydrides on the local notch tip strain field and characterize the internal strains in the hydrides themselves.

Pb-Free Solders and Emerging Interconnect and Packaging Technologies: Microstructure, Intermetallics, Whisker (II)

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

Thursday AM — Room: 204
February 18, 2010 — Location: Washington State Convention Center

Session Chairs: John. W. Osenbach, LSI Corporation; Sinn-Wen Chen, National Tsing Hua University

8:30 AM
Effects of Current Density on the Crystallographic Texture of Sn Based Electrodeposited Films Containing Cu and Pb: *Aaron Pedigo*[1]; Pylin Sarobol[1]; Peng Su[2]; John Blendell[1]; Carol Handwerker[1]; [1]Purdue University; [2]Cisco Systems, Inc

Tin whisker growth is a reliability concern for lead-free electronic systems. Current whisker testing is performed with regards to JEDEC standards but the output from these tests only reports if a film is or is not whisker prone. An understanding of the mechanism of whisker formation is necessary to develop whisker mitigation strategies. Other material properties should be measured to engineer electrolytes and plating processes that decrease the propensity to whisker. In this work, the effects of electrolyte chemistry and current density during plating on texture and hillock and whisker growth were evaluated. Full pole figure analysis was performed using XRD with GADDS. EBSD was also performed to compare local texture to the macroscopic texture. Results show that the addition of Pb in the electrolyte causes drastic changes in crystallographic texture. The texture effects from Pb could be recreated in lead free electrolytes by changing the current density.

8:45 AM
Interfacial Reaction and Microstructure Variation in the Liquid Reaction of Sn-xAg-Cu Solders on Cu-yZn Substrates: *Chi-Yang Yu*[1]; Jenq-Gong Duh[1]; [1]National Tsing Hua University

This study aims to investigate the liquid reaction of Sn-xAg-0.5Cu (x= 1 and 3 wt.%) solders on different Cu-yZn (y= 0, 15 and 30 wt.%) substrates at 250 oC for 30 s, 2 and 10 min, respectively. Cu and Zn atoms would dissolve from Cu-xZn substrates into molten solders during reflow. Under this condition, Cu6Sn5 was the dominating intermetallic compound (IMC) formed at the Sn-xAg-Cu/Cu-yZn interface. The composition of the Cu6Sn5 and other IMCs were altered with various solder joints and reflow time. Besides, IMCs growth rate was affected by the Zn concentration at the interface. In addition to interfacial reaction, the microstructure evolution and phase formation inside the Sn-3Ag-Cu and Sn-1Ag-Cu solders were correlated to the elemental distribution. Based on these results, the interaction between Ag content (x) in solder and Zn content (y) in substrate will be probed and discussed.

9:00 AM
Interfacial Reaction between Sn-Ag-Cu Solder and Cu Base Metal Using Laser Soldering Process: *Hiroshi Nishikawa*[1]; Noriya Iwata[1]; Tadashi Takemoto[1]; [1]Osaka University

With the miniaturization of electronic productions and the use of heat sensitive electronic components, the traditional reflow soldering process often has difficulties. As an alternative soldering process, the laser soldering process has been recently proposed. The laser soldering process brings several advantages in terms of localized heating, rapid rise and fall in temperature, non-contact and easily automated process. Therefore, in this study, the characteristics of the laser soldering process were investigated to especially clarify the effect of the heating method on the formation and growth of an intermetallic compound (IMC) at the interface between Sn-Ag-Cu solder and a Cu base metal and the microstructure of the solder after heating. The results show that the rapid rise and fall in temperature strongly affected the IMC at the interface and the IMC thickness for the laser soldering process was thinner than that for the traditional reflow soldering process.

9:15 AM
Microstructure and Orientation Evolution Study on Sn-Ag-Cu Solder Joints as a Function of Position in Ball Grid Arrays Using Orientation Image Microscopy: *Tae-Kyu Lee*[1]; Kuo-Chuan Liu[1]; Bite Zhou[2]; Thomas R. Bieler[2]; [1]Cisco Systems, Component Quality and Technology Group; [2]Chemical Engineering and Materials Science, Michigan State University

The microstructure evolution of Sn-Ag-Cu solder alloy joints are observed during thermal cycling, focused on Sn grain orientation in ball grid array (BGA) packages with different die sizes. Thermally cycled BGA packages after various pre-conditions with 196 full array solder joints are used in this study. Each selected package is polished to view the solder joints from the top by using an Orientation Imaging Microscopy. The observations reveal different patterns of single and multi-grained Sn microstructure distribution and Sn c-axis orientation for each solder joint as a function of position in the package depending on their pre-condition and thermal cycle history. The overall percentage of the single grain oriented solder joints is reduced after thermal cycling with a faster rate after 150°C aging condition compared to lower aging temperature. The difference of the distribution of individual grain orientations and evolution of those orientations during thermal cycling are discussed.

9:30 AM
Stress and IMC Growth in Annealed and Reflowed Sn-Cu Bilayers and Their Relation to Whisker Kinetics: *Nitin Jadhav*[1]; Gordon Barr[2]; Eric Chason[1]; [1]Brown University; [2]EMC Corporation

Though annealing and reflowing in Pb-free Sn have been recognized as effective methods to impede whisker formation, little is known about the fundamental mechanisms that make them work. We have done studies to understand how different heat treatments (annealing, reflow, and annealing followed by reflow) affect the stress development in the Sn layers and growth and morphology of the intermetallic (IMC), which are the key parameters controlling whisker formation. In order to quantify the nucleation kinetics we have measured the whisker density using an optical method. Our results show how the heat treatment results in IMC formation which is more continuous and uniform compared to the as-deposited sample. This impedes whiskering in two ways: the IMC layer is an effective diffusion barrier that slows down the IMC growth kinetics and the smoother morphology creates less stress in the overlayer for the same volume of IMC as in the as-deposited sample.

9:45 AM
Nucleation and Solidification of Sn in Pb Free, SnAgCu Solder Joints: *Babak Arfaei*[1]; Yan Xing[1]; Eric Cotts[1]; [1]Binghamton University

The replacement of eutectic Pb-Sn with near eutectic Sn-Ag-Cu to create Pb free solder joints has provided a number of challenges. Ag and Cu are much less effective than Pb in promoting solidification of Sn, so pronounced undercooling, and thus rapid solidification effects on solder joint microstructure are observed in standard procedures. Furthermore, six-fold, cyclic growth twinning of Sn during solidification from the melt is generally observed in Sn-Ag-Cu solders.

This study examines variations in solder joint microstructure resulting from changes in solidification pathways. The solder impurity content, sample size and solder joint properties, such as substrate metallization, are varied. Both variation of nucleation rates of Sn from the Sn-Ag-Cu melt, and of resultant Sn grain solidification morphologies, are reported. Studies of the failure of Sn-Ag-Cu solder joints are discussed in the context of these different Sn grain morphologies.

10:00 AM Break

10:15 AM
Mitigation of the Growth of Tin Whiskers by Surface Treatments: *Chien-Hao Su*[1]; Albert T. Wu[1]; [1]National Central University

The growth of tin whiskers on lead-free finishes coated on the leadframes is a spontaneous process and contributed by stress generation and relaxation. A protective layer of tin oxide that grown on the surfaces is required for the formation of tin whiskers. The oxide layer prevents the relaxation of stresses that are built up due to the formation of intermetallic compounds. Cracks on the oxide served as weak spots that are essential for the protrusion of whiskers to release the stresses. This paper presents a new approach to mitigate the growth of tin whiskers. The sample surfaces were treated by etchant and polishing to greatly reduce the coherence of oxide. Tin oxide nanoparticles were sprayed on the "clean" surface to deliberately produce weak spots to enhance the relaxation of stresses. The results suggested that many short hillocks instead of long whiskers grown after performing surface treatments.

10:30 AM
Interfacial Reactions of Cu/Sn3.5Ag/Au Solder Joint under Electromigration: *Tsung-Chieh Chiu*[1]; Kwang-Lung Lin[1]; [1]National Cheng Kung University

In this study, a lead free Cu/Sn3.5Ag/Au solder joint under electromigration of 2.56×103 A/cm2 at 100° with various times was investigated. After 480 h of current stressing, the morphology of cathodic Cu electrode became rough which is due to the migration of Cu toward the anode side. The AuSn4 in the solder matrix near the Cu electrode tended to dissolve and released Au in the interfacial Cu6Sn5 to form (Cu,Au)6Sn5. The migration of Sn to the anode resulted in the formation of crack at the (Cu,Au)6Sn5/solder interface. As the Cu at the anode side, the thickness of IMC formed under electromigration is greater than that under isothermal aging. At the Au electrode, four types of IMC including AuSn4, AuSn2, AuSn and Au5Sn were sequentially formed at the interface regardless of the direction of electron flow under electromigration.

10:45 AM
The Relationship between Whisker Growth and Corrosion in Sn-3.0Ag-0.5Cu: *Keith Sweatman*[1]; Takashi Nozu[1]; J Masuda[1]; Masuo Koshi[1]; Tetsuro Nishimura[1]; [1]Nihon Superior Co., Ltd.

Corrosion has been identified as one source of the compressive stress recognized as a driver of whisker growth in high-tin alloys and in this paper the authors report a study directed at identifying the relationship between the extent of corrosion and whisker growth. Printed circuit coupons with an OSP finish were soldered with Sn-3.0Ag-0.5Cu using wave, reflow, and manual methods with a range of "no-clean" fluxes typical of current commercial practice and exposed for up to 3000 hours to 40°C/95%RH, 60°C/90%RH and 85°C/85%RH. As well as recording the location of whiskers, their density, and length as a function of time, the extent of corrosion of the solder was measured by cross-sectioning. While the environment proved to be the main controlling factor the incidence and growth rate of whiskers was found to vary with the soldering method, the flux type, and the geometry and could be correlated with the concomitant corrosion.

11:00 AM
Corrosion Enhanced Sn Whisker Growth: *John Osenbach*[1]; H. L. Reynolds[2]; G. Henshall[3]; R. D. Parker[4]; P. Su[5]; [1]LSI Corporation; [2]Sun Microsystems, Inc.; [3]Hewlett-Packard; [4]Delphi Electronics and Safety; [5]Cisco Systems

Sn whisker growth is affect by corrosion. We have found corrosion enhances whisker growth by lowering the effective activation energy for whisker growth. A theory based on excess, non-creep relaxed, oxidation induced strain was developed to explain the corrosion induced energy barrier lowering.

11:15 AM
Back-Stress Induced Single Crystal Hillock Growth in Unpassivated and Nanotwinned Copper Lines under Electromigration at Device Operation Temperature: *Hsin-Ping Chen*[1]; King-Ning Tu[1]; Lih J. Chen[2]; Chien-Neng Liao[2]; W.W. Wu[3]; [1]UCLA; [2]NTHU; [3]NCTU

Hillock growth has been observed in unpassivated and nanotwinned copper lines under electromigratin at normal device operation temperature of 100°C by using ultrahigh vacuum transmission electron microscopy. The formation of hillocks in the anode side implies that electromigration has caused a back-stress and also a localized stress gradient in the Cu line. From TEM analysis, the single crystal hillocks are larger than the grain size in the line and have facets. The growth direction of hillock is random and there is no preferred orientation.

11:30 AM
Microstructure Changes and Physical Properties of the Intermetallic Compounds Formed at the Interface between Sn-Cu Solders and Cu Substrate Due to Minor Additions of Alloying Elements: *Petr Harcuba*[1]; Milos Janecek[1]; [1]Charles University Prague

Several Sn-based alloys have been proposed recently as lead-free alternatives of Sn-Pb alloys. Sn-Cu alloy seem to be one of the most promising candidates with several enhanced properties which are achieved by additions of other elements. In this study the influence of alloying elements on the morphology of intermetallic compounds (IMC) formed at the interface of the liquid Sn-Cu solder and Cu substrate has been investigated. Minor additions of alloying elements, in particular Ni and P, were shown to improve soldering as well as other physical properties of the joints. The morphology and composition changes of the IMC layer formed during liquid solder/solid Cu substrate reaction in a wide range of temperatures and reaction times were investigated by scanning electron microscopy and energy dispersive X-ray analysis. The IMC layer growth kinetics is analysed using Arrhenius approach.

11:45 AM
Reaction between Sn and Electroplated Cu Foils with Different Orientation: *Tzu Sung Huang*[1]; C. Y. Liu[1]; Hua-wei Tseng[1]; Yu-Hsiang Hsiao[1]; Cheng Tze Liu[1]; [1]National Central University

The binary Cu/Sn soldering system is the most important joint system in the current IC packaging. In this thesis, we will study the correlation between the microstructure of Cu substrate (Cu grains size and preferred orientation) and the interfacial reaction (Cu-Sn compound formation and Kirkendall voids distribution). Cu substrates with different orientation are prepared by electroplating, and then reflow solder balls on the electroplated Cu substrates. After that, aged the Sn/Cu samples under 150°. In this investigation, the electroplated Cu were performed by metallurgical examination, XRD and FIB analysis to examine the grain size morphology, preferred orientation and Kirkendall voids distribution. The experimental results indicated that the Cu3Sn thickness of Cu substrate with the (Random) plane is thicker than that with the (111) and (220) planes. In addition, there was almost no Cu3Sn growth in (111) and (220) after 2000 hrs aging.

Polymer Nanocomposites: Fabrication, Characterization, Modeling and Applications

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

Thursday AM Room: 309
February 18, 2010 Location: Washington State Convention Center

Session Chairs: Jiahua Zhu, Lamar University; Wei Chen, University of Southern California

8:30 AM Introductory Comments

8:35 AM Invited
Negative Permittivity in Polymer Nanocomposites: Influences of Size Distribution of Carbon Nanofiber Networks: *Bin Li*[1]; Weihong Zhong[1]; [1]Washington State University

A polymeric "single negative permittivity metamaterial" was successfully fabricated from the non-metallic materials, polyetherimide (PEI) and carbon nanofibers. The determinant structure in the polymer nanocomposites was the continuous 3D network composed of imide chains wrapped upon long CNFs (CNF agglomerates), which is equivalent to the thin metallic wires in the J.B.Pendry Model. In this study, the low power ultrasonic treatment was applied to disentangle the large CNF agglomerates and consequently reduce the size of the CNF agglomerates and their related distribution. The results showed that the size of CNF agglomerates exerts strong influence on the occurrence of negative permittivity. A qualitative relationship between size/size distribution and negative permittivity of PEI/CNF nanocomposites was established.

9:05 AM

Crystallization Behavior of Polymer Nanocomposites: Influence of Pressure and Nanoparticles: *Qiang Yuan*[1]; Jinesh Shah[1]; Juan Chen[1]; Yang Yang[1]; Devesh Misra[1]; [1]University of Louisiana

The objective of the presentation is to elucidate the basic physical mechanisms underlying the evolution of hierarchical structures and phases during pressure-induced crystallization of polymers containing dispersion of nanoparticles. High pressure crystallization enables structural characteristics such as high crystallinity and preferential phase selection in polymer nanocomposites. The phase selection in the polymers is normally dictated by pressure and temperature, however, the introduction of nanoparticles can dramatically alter the kinetics of the formation of the phases via nanoparticle interface driven nucleation. Thus, by controlling pressure and crystallization temperature, a high degree of phase selection and structural control may be achievable, which has profound effect on mechanical properties.

9:25 AM

Effect of Melt Flow Rate on the Properties of Polypropylene/Bentonite Nanocomposites: Tatianny Alves[1]; Laura de Carvalho[1]; *Eduardo Canedo*[1]; Pamela Cipriano[1]; Vanize Fernandes[1]; [1]UFCG

Polymer nanocomposites have several advantages over conventional microcomposites, among which is the fact that similar or better properties can be obtained at very low loadings (1-5%). Layered silicates such as those present in bentonite clays are some of the most useful loads. Melt compounding with organically modified clays is the preferred method to prepare nanocomposites based on non-polar matrices such as polyolefins. In this work, nanocomposites made with two polypropylene homopolymers having very different melt flow rates (10 and 40 g/10min) and 1% local bentonite clay, organofilized with hexadecyl trimethyl ammonium bromide in our laboratories, were prepared by melt compounding in a single-screw extruder fitted with mixing elements. Results show that intercalated structures were obtained with both matrices. A larger increase in interlayer spacing was observed for the compounds made with the more viscous, i.e., lower MFR polymer.

9:45 AM

Synthesis, Structure and Properties of a Novel Hybrid Bimodal Network Elastomer with Inorganic Cross-Links: *Jinesh Shah*[1]; Qiang Yuan[1]; Juan Chen[1]; Yang Yang[1]; Devesh Misra[1]; [1]University of Louisiana

A novel hybrid bimodal network elastomer was synthesized with high strength-high ductility combination involving utilization of functionalized nanocrystalline titania as short-chain cross-links between neighboring elastomer chains. Silicone rubber is selected as the model elastomer. The short-chain cross-links are acrylic acid functionalized nanocrystalline titania that are an integral component of bimodal network structure of the elastomer. To delineate and separate the effects of functionalization from nanoparticle effects, a relative comparison is made between silicone rubber-titania nanocomposite (i.e. containing dispersion of titania as a reinforcement filler) and silicone rubber-titania hybrid network elastomer (i.e. titania as short chain cross-links). The basic physical mechanisms that govern elastic recovery in hybrid bimodal network elastomer with short chain cross-links of functionalized nanocrystalline inorganic particles are discussed.

10:05 AM

Modification of Nanocrystal-Polymer Composite Electrolyte by Ethelene Glycol for Dye-Sensitized Solar Cell: *Yang Ying*[1]; Guo Xueyi[1]; [1]Central South University

A quasi-solid-state dye-sensitized solar cell (DSSC) employing poly (ethylene oxide)-poly (vinylidene fluoride) (PEO-PVDF) gel electrolyte was modified by ethanol and glycol. The performance of additive-modified electrolyte was studied by Fourier transform infrared (FTIR), differential scanning calorimetry (DSC) and viscosity measurements. The conductivity of the electrolytes and the corresponding performances of the DSSC were also studied. The experiments exhibit that 3.1% ethanol modified electrolyte shows an increase of the connected ion transport networks in the electrolyte, leading to an improvement in energy-conversion efficiency from 4.4% (unmodified DSSC) to about 5.3% and an increase in stability from 130 to about 500 hours in room temperature. However, compared to ethanol modification, the same amount of gycol addition into the electrolyte causes little improvement in both conductivity and cell performances. This may be due to the formation of an polymer aggregates in the electrolyte, which inhibits the ion transport in the electrolyte.

10:25 AM Break

10:40 AM

Nanoscale Near-Surface Deformation in Polymer Nanocomposites: *Qiang Yuan*[1]; Jinesh Shah[1]; Yang Yang[1]; Juan Chen[1]; Devesh Misra[1]; [1]University of Louisiana

The objective of the presentation is to elucidate the nanoscale near-surface deformation response of two polymer nanocomposite systems with significant differences in ductility during nanoscratching with a Berkovich indenter. An accompanying objective is to investigate the commonality in surface deformation behavior between nano- and microscale deformation to reinforce the underlying fundamental principles governing surface deformation. An understanding of surface deformation response is accomplished through determination of physical and mechanical properties, structural characterization and electron microscopy analysis of surface deformation tracks and residual plastically deformed structures. The deformation behavior is described in terms of physical and mechanical properties of materials notably percentage crystallinity and elastic recovery.

11:00 AM Invited

Formation and Structural Characterization of Potassium Titanates and the Lattice Potassium Reactivities: Qiang Wang[1]; *Zhanhu Guo*[1]; Jong Shik Chung[2]; [1]Lamar University; [2]POSTECH

Potassium titanates (K2Ti2O5, K2Ti4O9 and K2Ti6O13) are synthesized by solid state method. Their structures and morphologies are characterized by X-ray diffraction, Raman spectra and scanning electron microscopy. The binding energies of K, Ti and O in potassium titanates are then evaluated by X-ray photoelectron spectroscopy and compared with those in K/TiO2. Finally the lattice potassium reactivities are evaluated by NO2 adsorption and ion exchange in Co(NO3)2 solutions. It is found that the binding energy of K in K2Ti2O5 is much higher than those in K2Ti4O9 and K2Ti6O13, and because of which, it shows quite different catalytic performances. Compared with other potassium titanates, only K2Ti2O5 shows NO2 adsorption activity and the K in K2Ti2O5 is much easier to be exchanged out.

11:20 AM

Catalytic Reduction of Nitrates Using Modified Double Layered Hydroxides: *Jewel Gomes*[1]; George Irwin[1]; Kamol Das[1]; Manish Rahate[1]; Doanh Tran[1]; David Cocke[1]; [1]Lamar University

Layered Double Hydroxides (LDHs), such as green rust and hydrotalcites, are a group of anion-exchangeable materials containing mixed metal hydroxides similar to brucite. They have relatively weak interlayer bonding compared to cationic clays resulting excellent ability to capture inorganic anionic contaminants, such as nitrates. With the increasing sources of nitrogen and nitrates from natural, agricultural, and man-made activities, nitrate contamination of groundwater is a common problem when surface water comes in contact with any source of nitrate. Existing nitrate (NO3-) treatment processes such as distillation, reverse osmosis, and ion exchange, are expensive and have inherent disadvantages. The aim of this study was to investigate the feasibility of catalytic removal of nitrate using modified LDHs formed by impregnition of transition metals. The study also included the characterization of modified LDHs using XRD, FTIR, SEM and Mössbauer spectroscopy. Thermal degradation and flame retardant effect of the nano-LDHs were also studied.

11:40 AM

Molecular Dynamics Simulation of Diffusion of Atmospheric Penetrates in Polydimethylsiloxane (PDMS) and PDMS-Based Nanocomposites: *Alex Sudibjo*[1]; Douglas Spearot[1]; [1]University of Arkansas

Molecular dynamics simulations are used to study the nanoscale mechanisms associated with diffusion of small atmospheric penetrates in polydimethylsiloxane (PDMS) and PDMS-based nanocomposites with metal nanoparticle inclusions. Specifically, diffusion constants and activation energies are computed for methane, nitrogen and oxygen penetrates in PDMS and PDMS-based nanocomposites. PDMS is modeled within the molecular dynamics framework using both united-atom and all-atom interatomic potentials; the accuracy of each model and its ability to capture structural aspects of PDMS, including bulk densities and radius of gyration, is evaluated. Diffusion coefficients are computed via mean-squared displacements of the atmospheric penetrates. MD simulations provide a detailed understanding of how penetrate species, temperature, nanoparticle size and distribution influence the diffusion flux through the nanocomposite. These calculations are necessary to interpret experimental results for a MEMS-based corrosion sensor, where metallic nanoparticles are embedded within a PDMS matrix.

12:00 PM
Metallization of Platinum on Polyimide as Counterelectrode for Flexible Dye-Sensitized Solar Cells: *Sheng-Jye Cherng*[1]; Chih-Ming Chen[1]; [1]National Chung Hsing University

The counterelectrodes of flexible dye-sensitized solar cells (DSSCs) are usually fabricated by sputtering a catalytic platinum (Pt) layer on flexible transparent conductive polymer substrate (ITO/PEN). However, sputtering is not a cost efficient method which restrains its applications. Therefore, development of a low cost method of depositing Pt for DSSCs is an important issue. In this talk, we demonstrate a simple and low cost method of growing Pt nanoparticles on polyimide. Four point probe analysis reveals the nonconductive polyimide becomes electrically conductive after surface metallization of Pt. DSSCs employing the Pt-coated polyimide as the counterelectrodes were assembled and their photovoltaic performances were measured.

Processing Materials for Properties: Polymers, Ceramics and Glasses

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

Thursday AM — Room: 617
February 18, 2010 — Location: Washington State Convention Center

Session Chairs: Stuart Maloy, Los Alamos National Laboratory; Mychailo Toloczko, Pacific Northwest National Laboratory

8:30 AM Keynote
Transparent Ceramics by Spark Plasma Sintering of Oxide Nanopowders: *Rachman Chaim*[1]; Zhijian Shen[2]; Claude Estournes[3]; [1]Technion - Israel Institute of Technology; [2]Stockholm University; [3]CIRIMAT et Plateforme Nationale CNRS de Frittage Flash

Spark plasma sintering (SPS) was used for superfast densification of ceramic nanopowders. Simultaneous application of pulsed dc currents and load are the necessary conditions for rapid and full densification of ceramic nanopowders by SPS. Nanopowders of MgO, YAG and Y2O3 were densified using SPS at different temperatures, pressures and durations. Nanocrystalline MgO and YAG powders were densified to optical transparency at distinctly different homologous temperatures (0.3Tm for nc-MgO and 0.7Tm for nc-YAG). Dense Nd-YAG and Y2O3 specimens were translucent with micrometer grain size. Analysis of the density and grain size evolution versus the SPS parameters showed that densification of these nanopowders proceed either by plastic deformation, grain-rotation coalescence and sliding, aided by softening of the particle surfaces or by accelerated surface diffusion. These may be followed by normal grain growth. The active densification mechanism depends on the changes both in the mechanical and electrical properties of the ceramic with temperature.

9:00 AM
Direct Laser Deposition of Bulk Metallic Glasses: *Hongqing Sun*[1]; Pete Collins[1]; Hamish Fraser[1]; Katharine Flores[1]; [1]The Ohio State University

Bulk metallic glasses (BMGs) have attracted tremendous attention as structural materials because of their remarkable mechanical properties. However, the critical cooling rates required to produce an amorphous atomic structure limit the dimensions of as-cast BMG components and therefore restrict their widespread use. As a layer-by-layer additive process with localized heat input and inherently rapid cooling, direct laser deposition provides the potential opportunity to produce non-equilibrium or amorphous structures that exceed the as-cast dimensional limit. In the present work, we use the Laser Engineering Net Shaping (LENS™) process to deposit pre-alloyed Zr-based metallic glass forming powders. A continuous amorphous layer was achieved with optimization of the processing parameters. However, the accumulated heat input during multi-layer deposition results in the crystallization at the bottom of the deposit. To address this, we investigate the thermal history of the deposit and substrate using a combination of finite element modeling and in-situ thermal imaging.

9:20 AM
Microscopic Study of Slags from a Secondary Lead Blast Furnace: *Fumito Tanaka*[1]; Yusuke Kimura[1]; Mikio Watanabe[2]; [1]Mitsubishi Materials Corp.; [2]Hosokura Metal Mining Co., Ltd.

Hosokura Metal Mining Co., Ltd. processes spent lead-acid battery to produce electrolytic lead, while leaving acceptable influences on the environment. The company derives noticeable competitiveness from proven technologies for operating the blast furnace, which was developed jointly with Mitsubishi Materials Corp. Emerged businesses to recycle various lead-bearing materials have also been enhancing the bullion production. Processing lead-bearing materials, however, impacts on the slag chemistry or energy balance of the blast furnace, thereby misleading the operators occasionally. Microscopic examination of slag samples from the blast furnace revealed the metallurgical cause of the operational difficulties and helped to identify secondary materials whose feeding rate should be optimized. Among impurities included in secondary materials, the present paper will focus on the metallurgical impact of alumina and soda. It will also discuss the furnace controls under the influence of alumina and soda, applying slag chemistry of the state of the art.

9:40 AM
Particle Size Distribution of Natural Montmorillonite Clay Using Dispersion Analysis: *Morgan Reed*[1]; Gary Beall[2]; David Cocke[1]; Jewel Gomes[1]; [1]Lamar University; [2]Texas State University

The particle size and distribution of suspensions of clays are of considerable interest to many industrial processes including oil-well drilling, environmental abatement, polymer nanocomposites, and nanoflake catalysts. Although exploration of the interactions between montmorillonite clay with water-ethanol mixtures was studied before, particle sizing drew particle attention in the realm of nanotechnology due to particle-particle interaction and its role in distribution and sedimentation. In this study, the particle size was determined by employing a dispersion analyzer utilizing extinction and transmission profiles. The particle size distribution of montmorillonite particles, dispersed in a water-ethanol mixture, was obtained by analyzing the light transmission at a defined constant position with the measured time. This method of analysis was used for its robust accommodation of all types of suspensions with broad size distributions. The competitive behavior between ethanol and water molecules for active sites located at clay particle edges was also discussed considering particle size variation.

10:00 AM
Study of Properties of Spinels, Obtained by Hydrothermal Synthesis: *Oscar Restrepo*[1]; Leidy Jaramillo[1]; Ernesto Baena Murillo[1]; [1]National University of Colombia

This study provides an analysis of the properties of spinels Fe(1-x)Zn(x)Cr2O4 obtained by hydrothermal synthesis. Experiments were conducted where changes were made to the pH, the concentration of precursor salts and the type of iron salt used. The response variables analyzed were the distribution of phases, color, particle size distribution, chemical composition and shape of particles. The methods used to characterize the spinels obtained were by X-ray diffraction (XRD), UV-VIS-NIR spectroscopy, scanning electron microscopy (SEM), energy dispersion X-ray analysis of (EDX) and thermal analysis (DTA/TGA). Results are compared with a commercial product obtained by traditional method of solid state synthesis at high temperature. It is hoped that this study will serve as a technical option for the development of alternate routes for spinels production so as to provide environmental benefits, economic and technology compared to traditional methods.

10:20 AM
Research on the Performance of Environment-Friendly MgO-CaO-ZrO2 Refractories: *Caiyun Lu*[1]; Min Chen[1]; Jingkun Yu[1]; Zhongqiang Sun[2]; [1]Northeastern University; [2]Northeastern University Institute of Metallurgical Technology Co., Ltd

Considering MgO-Cr2O3 refractories used in the alkaline environment led environmental problems caused by hexavalent chromium pollution, MgO-CaO-ZrO2 refractories is a new type refractories for substitution of MgO-Cr2O3 refractories using in secondary refining vessels in metallurgical industries for its excellent properties as well as environment-friendly features. In the present work, Micro-ZrO2 and Nano-ZrO2 were used as additives applied in MgO-CaO refractories to respectively investigate their improvement on performance of MgO-CaO refractories. The results showed that the densification of the MgO-CaO refractories was appreciably promoted when a small amount of ZrO2 was added, the thermal shock resistance and slaking resistance of the MgO-CaO refractories could be appreciably improved with a small amount of ZrO2 addition. The effect of nano-sized ZrO2 additive on densification, thermal shock resistance and slaking resistance was more obvious than micro-sized one. The Penetration index of MgO-CaO refractories was significant reducted as the amount of nano-sized ZrO2 additive increased.

10:40 AM Break

10:50 AM
Synthesis of Spinels by Thermal Spray Flame: *Oscar Restrepo*[1]; Ernesto Baena Murillo[1]; [1]National University of Colombia

The formation of spinels Fe(1-x)Zn(x)Cr2O4 by thermal spray flame synthesis using iron (Fe2O3), zinc (ZnO) and chromium (Cr2O3) oxides as precursors is studied. It is evaluated the influence of two process operating parameters, O2/C2H2 ratio and pressure of those combustion gases, by X-ray diffraction (XRD), UV-VIS-NIR spectroscopy, scanning electron microscopy (SEM), energy dispersion X-ray analysis of (EDX) and thermal analysis (DTA/TGA). Changes in reflectance spectra of pigments obtained by this non-conventional method are related to the identified phase transformations, crystallinity and the spatial arrangement of cations. Results are compared with a commercial product obtained by traditional method of solid state synthesis at high temperature. This alternative production method present advantages as efficiency improvement of process and product, because of reductions in energy consumption and byproducts generation, as well as reducing environmental impacts.

11:10 AM
Novel Forming Techniques in Fabrication of Powder-Based Metals via Current Activated Tip-Based Sintering (CATS): *D. Elting*[1]; E. Villar[1]; K. Moon[1]; S. Kassegne[1]; K. Morsi[1]; [1]San Diego State University

Bulk powder-based products that are fabricated using spark plasma sintering are completed in significantly shorter times and lower temperatures compared to a conventional sintering process. This paper discusses novel techniques in current activated tip-based sintering (CATS) where current activation is applied "locally" through a conductive tip to a powder bed or compact under the application of a forming pressure. Research includes simple and more complex small-scale artifact fabrication through the CATS process, the variables involved and their optimization, and the implications for macro as well as micro scale pressure assisted manufacturing processes. The processing-manufacturing for property relations is discussed.

11:30 AM
Effects of Sensitizer Length on Radiation Crosslinked Shape-Memory Polymers: *Taylor Ware*[1]; Walter Voit[1]; Ken Gall[1]; [1]Georgia Institute of Technology

Poly(methyl acrylate) (PMA) is blended with poly(ethylene glycol) diacrylate (PEGDA) of several molecular weights in various concentrations and exposed radiation. PEGDA sensitizes the radiation crosslinking of PMA. Minimum dosage for gelation decreases from 25.57 kGy for unblended PMA to 2.06 kGy for PMA blended with 10.00 mole% PEGDA. Increasing the length of the blended PEGDA molecule at a constant molar ratio increases the efficacy of the molecule as a radiation sensitizer as determined by the increase in gel fraction and rubbery modulus across dosages. However, at a constant weight ratio of PEGDA to PMA, shorter PEGDA chains sensitize more crosslinking because they have more reactive ends per weight fraction. Sensitized samples of PMA with PEGDA were tested for shape-memory properties and showed shape fixity of greater than 99%. Samples had a glass transition temperature near 28°C and recovered between 97% and 99% of the induced strain when strained to 50%.

11:50 AM
Radiation Crosslinked Polyacrylates with Shape Memory: *Walter Voit*[1]; Taylor Ware[1]; Ken Gall[1]; [1]The Georgia Institute of Technology

Shape-memory polymers (SMPs) are active smart materials with tunable stiffness changes at specific, tailored temperatures. Thermoplastic SMPs lose "memory" properties near melt temperatures and have large residual strains, while network (thermoset) SMPs fully recover, limiting device disfiguration. However the use of thermoset SMPs has been limited in mass-manufacture and commodity applications because low-cost plastics processing techniques like injection molding and blow molding are not possible with network polymers. In this study of thermoset SMPs, beyond adjusting the glass transition temperature (Tg) between 28 and 60°C and tuning the recoverable force between 0.5 and 13 MPa, a novel manufacturing process, Mnemosynation, is described. The customizable mechanical properties of traditional SMP are coupled with traditional plastic processing techniques to enable a new generation of mass producible plastic products with thermosetting shape-memory properties: low residual strains, tunable recoverable force and adjustable Tg.

12:10 PM
Synthesis of Polyamine PET for the Sulfate Ions Removal in Aqueous Solution: *Haiying Wang*[1]; Liyuan Zhang[1]; Liyuan Chai[1]; Meilan Li[1]; [1]Central South University

Polyamine PET was synthesized by condensation polymerization of epichlorohydrin and triethylenetetramine. FTIR, TG and SEM were used to character the PET product. The sulfate removal performance of PET in aqueous solutions was studied. The results showed that the product had strong thermo-stability and good sulfate ion removal capability. The sulfate ions adsorption of PET can bring into equilibrium within 30 min and 10 min respectively at neutral and acidic aqueous solutions containing 2.0 g/L sulfate ions. When the reaction maintained 30 min, the sulfate ions removal ratio can reach more than 99.0 % in aqueous solutions with the absorption capacity 180 mg/g or so.

Stochastic Methods in Materials Research: Stochastic Methods II: Property Prediction and Material Design

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

Thursday AM	Room: 614
February 18, 2010	Location: Washington State Convention Center

Session Chairs: Dallas Trinkle, University of Illinois Urbana-Champaign; Richard Hennig, Cornell University

8:30 AM Invited
Probabilistic Materials Science: Taking AIM: *Greg Olson*[1]; [1]Northwestern University

The systems approach to computational materials design has expanded in the past decade to encompass the full materials development and qualification cycle. The efficient control of minimum property allowables has demanded a major departure from traditional data-driven empirical statistical methods to a new mechanistic predictive science of probabilistic materials behavior. Under the DARPA-AIM initiative, multidisciplinary tools were integrated within the iSIGHT system to predict microstructure-based property variation resulting from six stages of manufacturing, demonstrating a novel modified Bayesian method in which a mechanism-based probability distribution is calibrated with minimal data by linear transformation. Employing iSIGHT sensitivity analysis tools in early alloy design, the AIM methodology has now been successfully demonstrated in the process optimization and qualification of the new Ferrium S53 corrosion-resistant aircraft landing gear steel. Enhanced models developed under the ongoing ONR/DARPA D3D Digital Structure consortium support process optimization for control of minimum fatigue properties based on distributed microstructure.

9:00 AM Invited

The Application of Bayesian Neural Network Modeling for the Prediction of the Tensile and Fracture Toughness Properties in a/ ß Titanium Alloys: *Santhosh Koduri*[1]; Vikas Dixit[1]; Peter Collins[1]; Hamish Fraser[1]; [1]The Ohio State University

The development of novel combinatorial methods based on Bayesian statistics to address the structure property relationships in commercially important materials is a valuable step towards the accelerated maturation of the materials. Non-linear data modeling tools such as neural networks with Bayesian framework have been used to predict the tensile and fracture toughness properties of Ti6Al4V at room temperature. The development of rules - based models necessitates population of extensive database consisting of the information about the composition and microstructural features to train and test the neural network models. These models have been successfully used to isolate the influence of the individual microstructural features on the mechanical properties, consequently guiding the efforts towards the development of more robust phenomenological models. The influence of critical microstructural features on tensile and fracture toughness properties has been investigated using the electron back-scattered diffraction and transmission electron microscopy.

9:30 AM

A Stochastic Simulation Study of the Role of Hierarchy in Crack-Initiating Microstructural Arrangements in Fatigue Lifetime Distribution: *Sushant Jha*[1]; Christopher Szczepanski[1]; James Larsen[2]; [1]Universal Technology Corporation; [2]US Air Force Research Laboratory

Recent research has revealed that the mean and the lower-tail of fatigue lifetime distribution show disparate rates of response to relevant microstructural and loading variables. This difference in responses, which controls the lifetime variability, is underlined by crack initiation in a hierarchical array of local microstructural arrangements. Here, we employ stochastic simulation to study this hypothesis of fatigue variability. Random, polycrystalline ensembles with given nominal grain size distribution and crystallographic texture were constructed using Voronoi Tessellation. The ensembles were then probed for the incidence of various critical microstructural arrangements. Probabilities of occurrence of such arrangements as a function of the heterogeneity level were calculated and correlated with the experimentally determined crack-initiating microstructural configurations and their frequency of producing failures in a titanium alloy. The effect of varying nominal microstructural attributes as they affect the probability of occurrence of a life-limiting crack-initiation condition was investigated.

9:50 AM Break

10:00 AM Invited

Multiscale Design of Solute-Strengthened Aluminum Alloys: *W. Curtin*[1]; G. Leyson[1]; L. Hector[2]; [1]Brown University; [2]GM Technical Center

The strengthening of alloys by the addition of solutes is well-established across a wide spectrum of metal alloys. The actual predictions of strengthening are based on approximate models of dislocation/solute interactions. Here, we develop a stochastic model for substitutional solute strengthening in fcc alloys, using concepts derived from early work by Labusch wherein the solute strengthening arises from favorable solute concentration fluctuations over some critical length determined by the fluctuations and the interaction energies. We then use first-principles methods to calculate the solute-dislocation interaction energies within the core of an edge dislocation in Al, and use these energies as input into the model to make nearly parameter-free predictions of solute strengthening. A rate-dependent thermal activation model is used to extend the model to finite temperatures and experimental strain-rates. The methodology is applied to Mg, Si, Cu, and Cr solute additions to Al, and the predictions are compared with available experiments.

10:30 AM

Multiscale Entropy Analysis of the Portevin-Le Chatelier Effect in an Al-2.5%Mg Alloy: *Apu Sarkar*[1]; P Barat[2]; P Mukherjee[2]; [1]Bhabha Atomic Research Centre; [2]Variable Energy Cyclotron Centre

Portevin-Le Chatelier (PLC) effect, observed in many dilute alloys of technological importance, is one of the widely studied metallurgical phenomena. It is a striking example of the complexity of spatiotemporal dynamics resulting from the collective behavior of dislocations. In uniaxial loading with constant imposed strain rate, the effect manifests itself as a series of repeated stress drops in the stress-time curve. The complexity of the PLC effect in Al-2.5%Mg polycrystalline samples subjected to uniaxial tensile tests is quantified. Multiscale entropy analysis is carried out on the stress time series data observed during jerky flow to quantify the complexity of the distinct spatiotemporal dynamical regimes. It is shown that for the static type C band, the entropy is very low for all the scales compared to the hopping type B and the propagating type A bands. The results are interpreted considering the time and length scales relevant to the effect.

10:50 AM

Using Eigenvalue and Information Theory Analysis to Predict Failure in Plastically Deformed Aluminum Sheet: *Mark Stoudt*[1]; Joseph Hubbard[1]; [1]National Institute of Standards and Technology

A recent study employed two approaches to characterize the apparent structure observed in strain localization maps constructed from surface topography data acquired from deformed aluminum sheet with scanning laser confocal microscopy. One used a conventional two-point autocorrelation analysis, and the other used information theory to analyze the eigenvalue spectrum associated with each strain map. While the results from the ACF analysis proved inconclusive, the information theory-based approach revealed two competing processes: one where the formation of structure is favorable and one where it is not. The crossover point can be regarded as a precursor to failure because once the dominant process shifts, the surfaces become metastable and the application of additional strain produces perturbations that trigger the failure event. The methodology for this approach and the potential impact on models used to predict limiting strains shall be presented and discussed.

11:10 AM Break

11:20 AM Invited

Probabilistic Polycrystal Model for Twin Nucleation and Propagation in Zr and Mg: *Carlos Tome*[1]; Irene Beyerlein[1]; Laurent Capolungo[1]; [1]Los Alamos National Laboratory

This work proposes a probabilistic approach for introducing twin nucleation and propagation effects in plastic deformation simulations of hcp metals. The elements of the model are based on a recent statistical study of twinning in pure Zr and pure Mg. This study provided insight on the correlation between twinning and: grain size, grain orientation, neighbor misorientation, and grain boundary length. A simulation algorithm for the model is proposed and implemented into the Visco-Plastic Self-Consistent (VPSC) polycrystal code. Simulation results for pure polycrystalline Zr and Mg deforming at 76 and 300 K , respectively, are compared to previous results using deterministic twin models and to experimental information about stress-strain response, texture evolution and twin fraction evolution.

11:50 AM

Predicting and Validating the Stochastic Effects of Microstructure on Polycrystal Elasticity and Plasticity: *Luke Brewer*[1]; Corbett Battaile[1]; John Emery[1]; [1]Sandia National Laboratories

The continuum mechanics necessary to describe the stress concentration and plastic deformation around bolt holes, voids, and crack tips is well developed. However, these continuum-based methods generally treat the material constitutive laws as deterministic functions. They do not include any way of representing the variability found in real materials microstructures; and therefore cannot predict the variability of the component response. We will discuss the early results of our efforts to represent material constitutive laws as probabilistic functions for use in component-level simulations. Brass produced at multiple grain sizes is being used as a model system for studying the change in microstructural variability and its effect on mechanical variability. The experimentally determined microstructures are converted into statistical representations from which many “statistically similar” microstructures can be generated and then are used to generate probabilistic property descriptions. For validation, a combination of in situ microscale experiments with simulations will be presented.

12:10 PM

Modeling Stochastic Interaction between Fatigue Damage Evolution and Random Heterogeneities: *Yibin Xue*[1]; [1]Utah State University

Cyclic small-crack growth may consume a large portion of fatigue life of certain components under certain cyclic loading conditions. Measurement of fatigue small-crack growth on the surface of smooth or notch specimens has evolved into a mature experimental technique. However, post data processing and model correlation for fatigue small-crack growth has not progressed in a parallel manner to the measurement technique. A new physics-based, mathematically precise fatigue small-crack growth modeling method is developed based on a multistage fatigue modeling scheme. The uncertainty in measurement errors and the effects of random variation of microstructural features on the small-crack growth were explored using Monte Carlo (MC) simulations. The stochastic interaction between microstructural features and the fatigue crack front is numerically explored. Fatigue damage incubation life is proven to be an essential quantity, both mathematically and physically. The proposed model is demonstrated using fatigue surface crack growth measurements of a due-phase Ti-alloy.

Sustainable Materials Processing and Production: Sustainable Technologies II

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

Thursday AM February 18, 2010 — Room: 2B — Location: Washington State Convention Center

Session Chairs: Jeffrey S. Spangenberger, Argonne National Laboratory; Tim Skszek, Magna Cosma Engineering

8:30 AM Introductory Comments

8:35 AM
Lightweight Structural Concrete Incorporating Volcanic Materials for Sustainable Construction: *Khandaker Hossain*[1]; [1]Ryerson University

This paper presents the development of lightweight concrete (LWC) incorporating pumice aggregate and volcanic ash (VA) based ASTM Type I blended cement (PVAC). Fresh and mechanical properties of LWC mixtures such as slump, air content, compressive strength, tensile strength, density and modulus of elasticity are described. The durability characteristics are investigated by drying shrinkage (DS), water permeability, mercury intrusion porosimetry (MIP), differential scanning calorimetry (DSC) and microhardness tests. The investigation suggests the production of LWCs incorporating blended PVAC and VPA having satisfactory strength/durability characteristics for structural applications. The use of PVAC induces the beneficial effect of reducing drying shrinkage and water permeability as well as refinement of pore structures and better interfacial transition zone (ITZ). Development of such non-expensive and environmentally friendly LWCs with acceptable strength and durability characteristics is extremely helpful for sustainable development and rehabilitation of volcanic disaster areas around the world.

9:00 AM
Mechanical and Chemical Development of Alkali Activated Slag Fine Aggregate Concrete by Design of Experiment (DOE): *Alexander Moseson*[1]; Aaron Sakulich[1]; Dana Moseson[2]; Ken MacKenzie[3]; M Barsoum[1]; [1]Drexel University; [2]Emerson Resources, Inc.; [3]Victoria University of Wellington

Alkali-activated cements (AACs) are an attractive alternative to ordinary portland cement as they have comparable performance and cost but little CO2 emission. The development of a ground, granulated, blast furnace slag-cement activated by soda ash (sodium carbonate), with a fine, granular limestone aggregate to form a fine-aggregate concrete will be presented. Mixture DOE was utilized, with analysis of compressive strength, hydraulic properties, and quantitative chemical products (by Rietveld analysis,) yielding valuable models of the system. This allows, amongst other things, a better understanding of mixture-component interactions, and the ability to optimize the system. Models for system responses will be presented and correlated. Successful formulations are hydraulic and cure at room temperature, with strengths as high as 40.7 MPa at 3 days, 64.5 MPa at 28 days and costs as low as ~ $33 USD/tonne for materials.

9:25 AM
Dissolution Behavior of Ru into the Na_2O-SiO_2-Al_2O_3 Slag System: *Hiroshi Shuto*[1]; Toru Okabe[1]; Kazuki Morita[1]; [1]University of Tokyo

Evaluation of dissolution loss of platinum group metals (PGMs) into molten slags is important in their pyrometallurgical recovery process. However, few research have been done on their solubilities into slags. In this study, dissolution behavior of Ru, one of the PGMs, into the Na_2O-SiO_2-Al_2O_3 slag system was investigated. About 1.5g of Na_2O-SiO_2-Al_2O_3 slags and 3g of Ru pellet were placed in Al_2O_3 crucible, and equilibrated at 1473±2 K in a resistance furnace for 18 hours. Partial pressure of O_2 was controlled to 10^{-4}-$10^{-2.5}$ atm by flowing a gas mixture of O_2 and Ar. After equilibration, the slag was subjected to chemical analysis to determine the Ru content. The solubility of Ru increases with increasing P_{O2}, and there is a linear relationship between $\log P_{O2}$ and log(ppmw Ru), with a slope of about 0.61, suggesting that Ru dissolves into the slags by oxidation as divalent or trivalent.

9:50 AM
New Process for Separation and Recovery of Platinum Group Metals: *Tsuyoshi Yukawa*[1]; Kazuki Morita[1]; Toru Okabe[1]; [1]The University of Tokyo

In order to develop an environmentally-sound materials recycling process, we investigated a new recycling process of platinum group metals (PGMs), particularly Rh, Ru, and Ir. The sustainable recycling process consist of a series of new pretreatment methods and a successive leaching step in aqueous solution without using any harmful oxidizing agent. During pretreatment, PGMs were reacted with Mg at 1193 K to obtain PGM-Mg alloys, which were then chlorinated using CuCl2 or other chlorination agents in the temperature range of 673–873 K. Finally, the obtained samples were dissolved in aqueous solutions of HCl or NaCl, which are free from strong oxidizer. The experimental results showed that valuable PGMs could be recovered by using a combination of the proposed pretreatment method and subsequent dissolution in HCl or NaCl solution. Currently, studies are underway for developing an effective pretreatment-dissolution combination for the successful recovery of PGMs.

10:15 AM Break

10:25 AM
Reductive Leaching Behavior of Valuable Metals from Spent Li-Ion Polymer Battery Cathode Material: *Jingu Kang*[1]; Jeong-soo Sohn[2]; Tae-hyun Kim[2]; Young-uk Kim[1]; Dong-hyo Yang[2]; Shun Myung Shin[2]; [1]Korea University of Science and Technology (UST); [2]Korea Institute of Geoscience and Mineral Resources (KIGAM)

Commercial trend of cathode material for Li-ion batteries, LiCoO2, is changing because of a shortcoming such as high prices, specific capacity having expanded to limit, raw materials falling in short, and not so safe. This study describes the leaching behavior of cobalt, lithium, nickel, and manganese from new type of spent cathode materials of Li-ion polymer battery. For extracting valuable metals from the active material, feasibility studies for leaching test were investigated in different parameters such as concentration of H2SO4, use of reductive or not, temperature, time, and agitation speed. The composition of powder was 19.8% Co, 7.3% Li, 19.9% Ni, and 18.3% Mn, respectively. Under the best leaching conditions (2.0 mol dm-3 H2SO4, 5vol% H2O2, 40°X, 100 g L-1 pulp density, 30 min, and 200 rpm), the leaching efficiency of cobalt, lithium, nickel, and manganese was over 99.5%, respectively.

10:50 AM
Materialization of Manganese by Selective Precipitation from Used Battery: *Shun Myung Shin*[1]; Jin-gu Kang[2]; Young-Uk Kim[2]; Tae-Hyun Kim[1]; Soo-Kyung Kim[1]; Jeong-Soo Sohn[1]; [1]Korea Institute of Geoscience & Mineral Resources (KIGAM); [2]Korea University of Science & Technology (UST)

MnO2 preparation by chemical methods is investigated for possible applications on materialization of manganese from used batteries. A preparation procedure was tested: reductive leaching and precipitation-oxidation by NaClO (single step-ClO). Leaching behavior of valuable metals with sulfuric acid and hydrogen peroxide was investigated in order to interpret the behavior of impurities. For extracting zinc and manganese from the used battery without other impurities such as copper, aluminum, and iron, the leaching tests were carried out. Leaching amount of zinc and manganese were 39.9 g/L and 30.3 g/L, under the leaching conditions at 1.0 mol dm-3 H2SO4, 3vol.% H2O2, 60°, 100 g L-1 pulp density, 1h, and 300 rpm. At the same time, the impurities in the leachate were Fe 0.5 ppm, Cu 2 ppm, and Al 1 ppm, respectively. As the result of XRD, we confirmed γ-MnO2 peaks. The purity of γ-MnO2 was 57.7% Mn, 0.01% Zn, respectively.

11:15 AM
Leaching Studies for the Recovery of Metals from the Waste Printed Circuit Boards (PCBs): *Manis Kumar Jha*[1]; Shivendra[2]; Vinay Kumar[1]; Banshi Dhar Pandey[1]; Rakesh Kumar[1]; Jae-chun Lee[3]; [1]National Metallurgical Laboratory (CSIR), India; [2]Indian Institute of Technology, Kanpur, India; [3]Korea Institute of Geosciences and Mineral Resources, South Korea

In view of recovery/ recycling of metals from PCBs, leaching studies were carried out from the PCBs containing Cu 17.05%, Ni 0.74%, Fe 1.74%, Pb 4.35% and Sn 8.32% using various acids like H2SO4, HCl and HNO3. Sulphuric acid was not found suitable leachant for the dissolution of metals from PCBs. However, hydrochloric acid selectively dissolved tin from the PCBs. The nitric acid was found to be effective lixiviant and 99.99% Cu, Fe, Ni and 36.66% Pb were leached out by 6M HNO3 at S/L ratio 100 g/L, and 90°C. The kinetic studies carried out with 2M and 4M HNO3 at 90°C showed "Ash diffusion control dense constant size-spherical particles" model. Similar kinetic model was observed with 6M acid concentration at 75°C. However, with an increase in temperature to 90°C, the kinetic model changed and was found to follow "Film diffusion control dense shrinking spheres".

11:40 AM Concluding Comments

The Vasek Vitek Honorary Symposium on Crystal Defects, Computational Materials Science and Applications: Grain Boundaries and Grain Boundary Engineering

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

Thursday AM — Room: 604
February 18, 2010 — Location: Washington State Convention Center

Session Chairs: Kevin Hemker, Johns Hopkins University; Diana Farkas, Virginia Tech

8:30 AM Invited
Modelling and Grain Boundary Engineering for High Performance Photovoltaic Polysilicon: *Tadao Watanabe*[1]; Kota Kido[2]; Sadahiro Tsurekawa[3]; [1]Visiting Professor, Northeastern University, Shenyang, China, formerly Tohoku University (Sendai,Japan); [2]YKK Corp., Japan; [3]Kumamoto University

Modelling of polycrystalline silicon with desirable grain boundary microstructure has been peformed to obtain useful information for future development of polysilicon sollar cell with high performance photovoltaic and electric properties by grain boundary engineering,on the basis of our recent experimental studies of structure-dependent electrical properties of individual grain boundaries in polysilicon (e.g.K.Kido, S.Tsurekawa and T.Watanabe; Phil.Mag.Letters, 85 (2005),41-49). Some recent attemps for Grain Boundary Engineering for high performance polysilicon by such as "unidirectional and rotational solidificationprocessing" T.T.Watanabe K.Kido and S.Tsurekawa; Mater.Sci.Forum, 558-559(2007),845-850) will be introduced, for fture development of high performance sollar cell polysilicon in the 21st century.

8:55 AM Invited
Atomic Characterization of Grain Boundary Networks in Poly- and Nano-crystalline Materials and Its Application: *Mo Li*[1]; Tao Xu[1]; [1]Georgia Institute of Technology

While single rain boundaries have been characterized and measured rather routinely for quite some time, following the pioneering work by Vitek, atomic characterization of grain boundary networks in poly- and nano-crystalline environment has been relatively unexplored to date. In this talk, we shall present a systematic method to build digital microstructures featured with the grain boundary networks of different characters. Contrasts to Gibbs' description of the mathematically abstract network, the grain boundary networks on atomic scale consist of topological entities with different dimensions and finite size. With the method, we could measure the thickness and area of a grain boundary, the length and diameter of a triple junction, and the volume of a vertex point, and their statistical or ensemble averages. Finally, we will show how those entities function in mechanical deformation in nanocrystalline materials, which is a special type of polycrystalline materials.

9:20 AM
The Role of Microstructure Scale and Morphology on Mechanical Behavior in FCC Metals: *Remi Dingreville*[1]; Corbett Battaile[2]; Luke Brewer[2]; Elizabeth Holm[2]; [1]Polytechnic Institute of NYU; [2]Sandia National Laboratories

One of the underlying principles of materials science is that materials properties can be deduced from the knowledge of its microstructural features. In particular, the sizes, shapes, orientation, line defects and connectivity of internal attributes are often critical in a material's response. However, many current approaches to simulating mechanical response lack this ability to adequately address so many factors at once.In this presentation, we will address two key aspects of this problem. First, we will present a dislocation-based constitutive model for the deformation of FCC metals in which the effects of the microstructure and its associated length scales are captured by a non-local crystal plasticity formulation. Second we will assess the role of microstructure's morphology by examining and comparing various microstructures (idealized and digitized micrographs) both at the macroscopic scale and the microscopic scale. This survey assesses the fidelity and sensitivity of the numerical model to the microstructural representation.

9:35 AM
Scale Invariance in Grain Misorientation Distribution: *Claude Fressengeas*[1]; Benoit Beausir[1]; Nilesh Gurao[2]; Satyam Suwas[2]; Laszlo Toth[1]; [1]University Paul Verlaine - Metz; [2]Indian Institute of Science

Grain misorientation is studied in relation with nearest neighbor's mutual distance using electron back-scattered diffraction measurements. The Misorientation Correlation Function is defined as the probability density for the occurrence of a certain misorientation between pairs of grains separated by a certain distance. Scale-invariant spatial correlation between neighbor grains manifests itself by a power law dependence of the preferred misorientation vs. intergranular distance in various materials after diverse strain paths. The scaling exponent is in the range of -2 ± 0.3 for high angle grain boundaries. It decreases in the presence of low angle boundaries or dynamic recrystallization, indicating faster decay of correlations. The correlations vanish in annealed materials, or when random assignment of grain pairs is performed. The results are interpreted in terms of lattice incompatibility and continuity conditions at the interface between neighboring grains. Grain size effects on texture development and the implications of such spatial correlations on texture modeling are discussed.

9:50 AM Break

10:05 AM Invited
Intermittency and Multiplication-Limited Flow in Microcrystal Deformation: *Dennis Dimiduk*[1]; Ed Nadgorny[2]; Chris Woodward[1]; Michael Uchic[1]; Satish Rao[3]; Paul Shade[4]; [1]Air Force Research Laboratory; [2]Michigan Technological University; [3]UES, Inc.; [4]UTC, Inc.

Current research seeks methods for coarse graining the ensemble dislocation response, especially when mean-field models fail. The microcompression method for single-crystal materials is contributing to understanding dislocation processes at micrometer scales and below. This work examines attributes of microcrystal deformation including strengthening and intermittency, for Ni and Mo, and LiF in as grown and irradiated conditions. The work examines dislocation mechanisms and dynamic processes for experiments and simulations. The studies suggest common attributes and incomplete interpretations for the observed behavior. They also suggest that a better understanding of both ensemble dislocation behavior and selected atomistic and dislocation core behaviors, as they pertain to dislocation multiplication, are necessary to complete the mechanistic views. One conclusion from the work is that a quantitative understanding of the time-dependent response may not be possible via current microcompression experiments because of the mismatch between time scales for the dislocation response and those for experimental observation.

10:30 AM Invited
Grain Boundary Plane Engineering: Model Experiments: *Pavel Lejcek*[1]; [1]Institute of Physics, AS CR

Recently, new concept of grain boundary plane engineering was proposed emphasizing the effect of the grain boundary plane orientation on the properties of polycrystalline materials (V. Randle, Acta Mater. 46 (1998) 1459). It is supposed that optimized polycrystalline material can also be produced by reorientation of the grain boundaries between existing grains during suitable annealing instead of forming completely new microstructure by recrystallization processes (P. Lejcek et al., Acta Mater. 51 (2003) 3951). In this contribution we show how the grain boundaries change their orientation from a high energy one to that possessing lower energy during thermal treatment of model samples: (i) bicrystals with free boundary; and (ii) tricrystals with one end of the boundary constrained at the triple junction.

10:55 AM
Molecular Dynamics Simulations of Atomistic Mechanisms for Grain Boundary Migration in [001] Twist Boundaries: Xinan Yan[1]; *Hao Zhang*[1]; [1]University of Alberta

Molecular dynamics simulations were performed to characterize atomic motions governing grain boundary migration in a series of twist boundaries. In particular, migrations of a S5, a S13 and a θ=40.23° general high angle [001] twist boundaries driven by stored elastic energy in an fcc Ni were investigated. The simulation results showed although four-atom shuffling motions were the predominant atomic motions in S5 twist boundary, they are intrinsic type of atomic motions and the correlation between individual four-atom shuffles are rather random than cascaded, as suggested by previous reports. Moreover, besides the four-atom shuffle, a more generalized cooperative string-like atomic motions was identified in all type of twist boundaries. Such a string-like motions tended to become stronger and more random as grain boundary losing its local symmetry. In addition, the activation energy for grain boundary migration is surprisingly well correlated with the average string length found in these boundaries.

11:10 AM
Ab Initio Investigation of Grain Boundary Cohesion in Al Alloys: *Shengjun Zhang*[1]; Oleg Kontsevoi[1]; Arthur Freeman[1]; Gregory Olson[1]; [1]Northwestern University

The embrittling and cohesion-enhancing effects of impurities on a Σ 5(012)[100] aluminum grain boundary are investigated by means of the full-potential linearized augmented plane-wave (FLAPW) method with the generalized-gradient approximation (GGA) formula within the framework of the Rice-Wang thermodynamic model. Analysis of the atomic and electronic structures identifies the roles of atomic size and the bonding behavior of the impurity with the surrounding Al atoms. The results show that He, H and Na are strong embrittlers, Zn is a weak embrittler, while Sc, B, Cu and Mg are cohesion enhancers. This work provides a fundamental electronic basis for stress corrosion behavior in Al alloys and provides quantitative parameters for the design of high strength Al alloys. Work supported by the AFOSR (grant No. FA 9550-07-1-0174) and the Ford-Boeing Nanotechnology Alliance at Northwestern.

11:25 AM
Role of Grain Boundary Character Distribution on Dynamic Recrystallization Using Monte Carlo Simulations: *Jared Stein*[1]; Megan Frary[1]; [1]Boise State University

Monte Carlo simulations are commonly applied to study microstructural evolution, including abnormal grain growth and recrystallization. Here, Monte Carlo simulations are used to study the effects of grain boundary character distribution on dynamic recrystallization. The initial stored energy is uniformly distributed and a constant strain rate is achieved by incremental increases in stored energy. The simulation tracks the grain size, special boundary fraction, and recrystallization fraction. Recrystallization rates vary with initial special boundary fraction and are compared to kinetic models. Similar to experimental results, a high percentage of grains that nucleate early in the simulation have special-boundary relationships with surrounding grains. As the simulation progresses, the orientation of nuclei becomes nearly random compared to surrounding grains. The simulations also predicted that the final special boundary fraction can be controlled by varying the strain rate. Once correlated with experimental results, the simulation can be used to investigate and refine hot-deformation processes.

11:40 AM
Development of a Microstructure Sensitive Model Which Shows Dislocation Patterning: *Alankar Alankar*[1]; Ioannis Mastorakos[1]; David Field[1]; [1]Washington State University

A dislocation density based crystal plasticity finite element model (CPFEM) is developed for aluminum which tracks dislocation densities on all octahedral slip systems. Based upon the kinematics of crystal deformation and dislocation interaction laws, dislocation generation and annihilation laws are modeled. It is shown that due to local deformation conditions e.g. deformation gradient, strain, and strain rate and orientation of each crystallite in a polycrystal, dislocation densities evolve heterogeneously. Description of dislocation densities is presented in form of pole figures along with evolution of crystallographic texture in idealized plane strain condition. Cross-slip of dislocations is modeled as a probabilistic event. The CPFEM model is calibrated for single slip and multi-slip deformation of pure aluminum using experimental stress-strain curves of pure aluminum single crystal from literature. Dislocation densities evolve as state variables in the model, leading to spatially inhomogeneous dislocation densities that show patterning in the dislocation structures.

11:55 AM
Dislocation Dynamics Simulations of Slip System Interactions and Dislocation Boundary Formation: *Benoit Devincre*[1]; Grethe Winther[2]; [1]CNRS-ONERA; [2]Risø National Laboratory

Analysis of fcc single crystal and polycrystal microstructures deformed in tension and rolling has established the combination of active slip systems and their interactions as the main factor controlling the crystallographic directionality of the dislocation boundaries. Five different classes of slip system interactions have been shown to give rise to different types of dislocation boundaries. As a first study, the case of duplex collinear slip is selected to investigate, by DD simulations, the fundamental dislocation mechanisms that control the formation and the stability of planar dislocation boundaries. For this case good agreement is found between the DD simulations of elementary dislocation-dislocation interactions and the experimentally observed dislocation boundary planes in grains/crystals with different crystallographic orientations and slip system activity. The results are promising for more general studies.

12:10 PM
On the Role of Dislocations during the Martensitic Transformation in NiTi Shape Memory Alloys: *Gunther Eggeler*[1]; Antonin Dlouhy[2]; [1]Ruhr University Bochum; [2]IPM Brno

NiTi shape memory alloys have fascinating properties. These rely on the martensitic transformation, a diffusionless phase transformation between a high temperature (B2) and a low temperature phase (B19'). Shape memory researchers have always been more interested in crystallography, in martensite variants and in phase transition temperatures than in dislocations. But dislocations are important in three respects. They are created during thermo mechanical processing of NiTi shape memory alloys to adjust certain properties (like tube or wire drawing followed by annealing). They are introduced when a SMA is trained for the two way effect. And they play a role during the martensitic transformation itself where they accomodated internal stresses (lattice invariant accomodation). The present contribution to the Vasek Vitek Honorary Symposium gives an overview on the different areas of overlap between dislocation plasticity and martensitic transformations. It then concentrates on how dislocations multiply during the martensitic transformation in NiTi alloys. And it finally outlines what effect dislocations have on the functional fatigue properties of shape memory alloys. Areas in need of further work are highlighted.

12:25 PM
Disclinations and Deformation of Hierarchically Twinned Martensite: *Peter Mullner*[1]; Alexander King[2]; [1]Boise State University; [2]Ames Laboratory

Shape-memory alloys deform via the reorganization of a hierarchically twinned microstructure. Twin boundaries themselves present obstacles for twin boundary motion. In spite of a high density of obstacles, twinning stresses of Ni-Mn-Ga Heusler alloys are very low. Neither atomistic nor dislocation based models account for such low yield stresses. Twinning mechanisms are studied here on a mesoscopic length scale making use of the disclination theory. In a first approach, a strictly periodic twin pattern containing periodic disclination walls with optimally screened stress fields is considered. Strict periodicity implies that the twin microstructure reorganizes homogeneously. In a second approach, a discontinuity of the density of secondary twins is introduced and modeled as a disclination dipole. The stress required for nucleation of this discontinuity is larger than the stress required for homogeneous reorganization. However, once the dipole is formed, it can move under a much smaller stress in agreement with experimental findings.

12:40 PM
Mesoscale Polycrystal Calculations of Damage Histories in Shock Loaded Metals: John Bingert[1]; *Davis Tonks*[1]; Veronica Livescu[1]; Curt Bronkhorst[1]; [1]Los Alamos National Lab

Dynamic damage evolution in metals is determined by both the stress loading history and the material microstructure. Important microstructural actors are the crystal grain boundary and twinning networks that directly promote void nucleation and deformation localizations that lead to void nucleation. The role of these networks in shock damage processes will be studied through polycrystal plasticity finite element calculations based on mesoscale microstructure from recovered samples. Results from copper and, possibly, tantalum samples will be addressed. The experimental loading will be the gas gun. The emphasis will be to understand the cause and effect in the damage evolution by supplying the calculated stress and strain histories, which are not measured in experiment. Correlations between void nucleation positions and microstructure will be sought.

The Vasek Vitek Honorary Symposium on Crystal Defects, Computational Materials Science and Applications: Grain Boundaries, Dislocations and Mesoscopic Modeling

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

Thursday AM — Room: 603
February 18, 2010 — Location: Washington State Convention Center

Session Chairs: Tadao Watanabe, Visiting Professor, Northeastern University, Shenyang, China, formerly Tohoku University (Sendai,Japan); John Bassani, University of Pennsylavnia

8:30 AM Invited
Shear Stresses, Dislocations and Grain Boundaries: *Kevin Hemker*[1]; [1]Johns Hopkins University

It is well known that shear stresses couple with dislocations and move them. It is also widely accepted that shear stresses can couple to low-angle tilt boundaries and move them. By contrast, high-angle grain boundaries are generally considered to be obstacles to dislocation motion. This talk will start with the effect of dislocation core geometry and non-Schmid stresses on the mobility of dislocations in intermetallic alloys, topics of which Professor Vitek has taught us much. Experiments on nanocrystalline thin films will then be used to highlight the fact that dislocation activity is fundamentally different in nanocrystalline metals and that shear stress-coupled grain boundary migration is manifest in room temperature grain growth and enhanced plasticity.

8:55 AM Invited
The Effect of Segregated Sp-Impurities on Grain-Boundary Embrittlement in Nickel: Monika Vsianska[1]; *Mojmir Sob*[1]; [1]Masaryk University, Faculty of Science

We have studied segregation and embrittling potency of sp-elements in the 3rd, 4th and 5th period (Al, Si, P, S, Ga, Ge, As, Se, In, Sn, Sb and Te) at the S5(210) grain boundary (GB) in fcc nickel and the segregation of these impurities at the (210) free surface (FS). Full relaxation of the geometric configuration of the GB and FS without and with impurities has been performed and the effect of impurities on the distribution of magnetic moments has been analysed. We determined the embrittling potency energy from the difference between the GB and FS binding energies on the basis of the Rice-Wang model; here a positive/negative value of this quantity means that the solute atom has the embrittling/strengthening effect on the GB. It turns out that all substitutionally segregated impurities studied are GB embrittlers in Ni.

9:20 AM
Multi-Time Scale Modeling of the Annealing of Radiation-Induced Defects at Tilt Grain Boundaries: Xian-Ming Bai[1]; Arthur Voter[1]; Richard Hoagland[1]; Michael Nastasi[1]; *Blas Uberuaga*[1]; [1]Los Alamos National Laboratory

We have used Molecular Dynamics (MD) and Temperature Accelerated Dynamics (TAD) simulations to investigate the annealing of radiation-induced damage near symmetric tilt grain boundaries (GBs) in copper over different time scales. The short-time (picoseconds) defect production stage is modeled by MD, and the resulting damaged structures are used as the input for long-time defect annealing studies in TAD simulations. Our simulations show that the defect annealing behavior in grain boundaries is quite different from that in single bulk crystals. The presence of the grain boundary affects the defect diffusion barriers significantly. The interaction between the grain boundaries and point defects results in new vacancy annealing mechanisms that help anneal the radiation-induced defects, significantly increasing the radiation tolerance of the material.

9:35 AM
Mesoscale Modeling of Particle Strengthened Interfaces: *Seth Wilson*[1]; A.D. Rollett[1]; [1]Carnegie Mellon University

Particle pinning remains the most practical way of controlling grain size and structure in materials. It is also critical to the phenomenon of abnormal grain growth (AGG), which is both a desirable process for certain production processes and an unwanted coarsening in other cases. Inmany materials, AGG is strongly correlated with temperatures near the solvus, when particles are dissolving. Computational modeling of this phenomenon must accurately reproduce particle-boundary, boundary-solute, and particle-solute couplings, as well as multi-junction constraints and topological transformations, at mesoscopic length scales in 3D, in a single simulation framework. To address this challenge, this work considers a novel modification of the level set method. A description of this modification and simulations demonstrating its versatility will be presented, including an exploration of boundary-particle interaction in the small-particle limit.

9:50 AM Break

10:10 AM Invited
Effect of Pre-Melting on Grain Boundary Properties: T. Frolov[1]; *Y. Mishin*[1]; J. W. Cahn[2]; [1]George Mason University; [2]National Institute of Standards and Technology

Pre-melting of grain boundaries can affect high-temperature behavior of materials. GB diffusion rates and response of GBs to applied shear stresses are examples of properties that can be strongly affected by GB pre-melting. We apply molecular dynamics simulations to show that these properties can also be used as sensitive probes of the pre-melted state of GBs. The self-diffusion coefficients of GBs and their triple junctions rapidly increase and approach the diffusivity of the bulk liquid phase as GBs develop liquid layers near the bulk melting point. In the same temperature range, the resistance of GBs to sliding rapidly drops to nearly zero, signifying the formation of a liquid layer.

10:35 AM Invited
Molecular Dynamics and Phase-Field-Crystal Studies of Grain Boundary Premelting in bcc Fe and fcc Ni: *David Olmsted*[1]; Dorel Buta[2]; Ari Adland[1]; Mark Asta[2]; Alain Karma[1]; Stephen Foiles[3]; [1]Northeastern University; [2]University of California, Davis; [3]Sandia National Laboratories

The premelting of grain boundaries is metallurgically important because of its effects on solidification and on high temperature processing. We have used molecular dynamics (MD) with embedded-atom potentials and the phase field crystal method (PFC) to study the premelting of <0 0 1> symmetric tilt boundaries in bcc Fe and fcc Ni. The critical misorientation angles for premelting in the two materials have been bracketed within four degrees for boundaries in MD on both ends of the misorientation range (boundary planes nearer to {1 0 0} and those nearer to {1 1 0}). A structural transition, distinct from premelting, is observed, both in MD and in PFC, in several of the boundaries, with the transition temperature depending sensitively on misorientation.

11:00 AM Invited
Lattice Geometry Effects on Ideal Shear Resistance and Dislocation Mobility: *Vasily Bulatov*[1]; Keonwook Kang[2]; Wei Cai[2]; [1]Lawrence Livermore National Laboratory; [2]Stanford University

Over its 75 years dislocation theory has repeatedly appealed to lattice geometry considerations, most notably to Frenkel's equation for the ideal shear resistance and to Vitek's concept of gamma surfaces. These two concepts inspired our recent attempts to relate dislocation mobility and crystal strength to the geometry of host crystal lattice. Based on a large number of accurate atomistic calculations we present two important observations: (1) that the common interpretation of Frenkel's equation relating shear resistance to the inter-planar spacing is incorrect and (2) that lattice resistance to dislocation motion is a discontinuous function of dislocation orientation. Analysis of atomistic calculations data for FCC and BCC model materials reveals that lattice geometry does indeed define both the ideal shear resistance and the line orientation dependence of dislocation mobility, but in ways that contradict the understanding prevailing in the literature. Finally, we describe implications of our findings for crystal shear strength.

11:25 AM
Applications of γ-Surfaces in Phase Field Modelling of Dislocations in Ni-Base Superalloys: *Vassili Vorontsov*[1]; Roman Voskoboinikov[1]; Catherine Rae[1]; [1]University of Cambridge

The "Phase-Field Microelasticity Theory" was used to simulate shearing of $L1_2$ ordered γ' phase precipitates by a/2<110> and a<112> dislocations. Incorporation of γ-surface data from atomistic simulations into the energy functional allows many complex core structures to be simulated on continuum scale. In addition to the conventional single-plane γ-surface, the concept of a two-plane "effective γ-surface" is introduced into the phase field model. This opens new dissociation pathways for the dislocations, which enables modelling of extrinsic stacking faults that form at elevated temperatures in superalloys. The model successfully demonstrates sensitivity of precipitate shearing mechanisms to variations in stress, precipitate geometry and dislocation character. Further potential applications of the model include its use as a tool, in conjunction with TEM, for measuring stacking fault and APB energies of complex alloy systems. Dislocation mobility during shear can be semi-quantitatively related to γ-surface topography, and input into creep models.

11:40 AM
Phase Field Modeling of Deformation Mechanisms in Ni-Base Superalloys: *Ning Zhou*[1]; Chen Shen[2]; Libor Kovarik[1]; Raymond Unocic[1]; Michael Mills[1]; Yunzhi Wang[1]; [1]The Ohio State University; [2]GE global

Plastic deformation in superalloys at service temperatures is often controlled by mechano-chemically or displacive-diffusionally coupled mechanisms of dislocation-precipitate interactions. For instance, chemical reordering may couple strongly to dislocation shearing of gamma prime precipitates and govern the rate of deformation. On the other hand, dislocation plasticity can also change the precipitate microstructure in so-called directional coarsening or rafting process. In this presentation, recent efforts in developing modeling approaches by integrating ab initio information such as the generalized stacking fault (GSF) energy with continuum phase field approaches, motivated and focused by experimental characterization, will be discussed. Examples will be presented to demonstrate the quantitative aspects of the microscopic phase field model in predicting critical stress for dislocation dissociation and superlattice extrinsic stacking fault (SESF) shearing of gamma prime precipitates, tension-compression asymmetry, and the effect of re-ordering kinetics on the rate of deformation. The work is supported by AFOSR under MAI program.

11:55 AM
Phase Field Simulations of Brittle Fracture in Composites with Spatially Varying Elastic Moduli: *Rajeev Ahluwalia*[1]; Weili Cheah[2]; [1]Institute of High Performance Computing; [2]Institute of Materials Research and Engineering

We perform phase field simulations of fracture in materials that are composites of a hard brittle component and a soft, less brittle component. The motivation of this study is to understand the fracture mechanisms in materials such as bone which are composites of a brittle mineral phase and a soft organic phase. We model this system by a material that has a spatially varying elastic moduli such that one component is hard and brittle where as the other component is soft and relatively less brittle. A phase field model is used to study crack propagation in such materials. It is demonstrated that a crack that initiates from a notch in the brittle phase stops on reaching the interface between the brittle and the soft phase. On increasing the strain, the crack propagates into the soft phase by branching. These results shed light on the toughening mechanisms in such composite materials.

12:10 PM
Phase Field Simulations of Elastic Deformation Driven Grain Boundary Migration in Copper: *Michael Tonks*[1]; Paul Millett[1]; Dieter Wolf[1]; [1]Idaho National Laboratory

Deformation can have a large influence on grain boundary migration, altering both the grain growth kinetics and the evolving grain structure. In this work, a phase field grain growth simulation is coupled with a linear elastic stress calculation to model deformation driven grain growth in copper. The model is verified by comparing the predicted behavior to atomic scale simulation results in bicrystals and analytical grain boundary migration expressions. Our simulations indicate that grains oriented such that they have a higher elastic stiffness in the load direction tend to have less stored elastic energy, and therefore tend to grow. The applied load does not change the exponent at which the average grain area grows, but it does alter the steady state grain size distribution and the final orientation distribution.

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

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

Thursday AM	Room: 203
February 18, 2010	Location: Washington State Convention Center

Session Chairs: Alejandro Strachan, Purdue University; Chunyu Li, Purdue University

8:30 AM Introductory Comments

8:35 AM Invited
Fundamental Processes in a Prototypical Organic Material: Nitromethane: *Donald Thompson*[1]; [1]University of Missouri-Columbia

Molecular organic crystals and liquids are ubiquitous, with usage ranging from drugs to energetic materials. Our understanding of chemical reactions in solids remains rudimentary at best. The main reason for this is that it is not possible to experimentally monitor events within a solid. Nevertheless, progress is being made, thanks in large part to theoretical modeling. Accurate modeling of chemistry requires a good understanding of the underlying fundamental physical processes. We have focused on a prototypical solid with the idea that a thorough understanding of it will help guide studies of more complex solids. We chose nitromethane because of its relatively small size yet complex molecular and crystalline behaviors. We have developed a force field that accurately predicts the structural and thermodynamic properties. We have most recently investigated post-shock behavior, including energy redistribution, in crystalline nitromethane. These and other recent results will be discussed.

9:05 AM
Elastic Deformation Mechanics of Cellulose Nanocrystals: Xiawa Wu[1]; Ryan Wagner[1]; Arvind Raman[1]; *Robert Moon*[2]; Ashlie Martini[1]; [1]Purdue University; [2]US Forest Service/ Purdue University

Cellulose nanocrystals (CNC) have great potential for polymer nanocomposite materials. However, a fundamental understanding of the CNC properties and their role in composite property enhancement is not currently available. To address this issue, we are developing atomic force microscopy (AFM) protocols combined with molecular dynamics (MD) and continuum modeling techniques that enable characterization of individual CNCs. AFM can be used to measure topography, pull-off force, stiffness and bending of CNCs, which are then related using the models to physical, chemical, mechanical and deformation properties, respectively. This paper outlines the development of a fully atomistic model of an individual CNC and its validation by comparison of predicted geometric, energetic, and elastic properties of the material to previous modeling results and experimental measurements.

9:25 AM

Break Down Assessment and Modeling of the Enthalpic Relaxation of Aging Glasses through a Combination of Experiment and Simulation: Chen Mao[1]; Sai Prasanth Chamarthy[2]; *Rodolfo Pinal*[3]; [1]Xenoport, Inc.; [2]Schering-Plough Research Institute; [3]Purdue University

The calorimetric glass transition encodes a wealth of information about the nature and structural behavior of organic molecular glasses. We present a DSC based investigation on the evolution of the thermal properties of glasses as a function of annealing time. A combination of experimental measurements and theoretical simulations produces a level of detail and accuracy not achievable by either method alone. The approach quantitatively discriminates between the effects of the glass forming properties of the material and the thermal history of the sample, including potential artifacts inherent to the choice of experimental method. Based on this approach, we propose an unambiguous definition of the time scale of the experiment, an important parameter that has remained vaguely defined at best. Using salicin as model compound, we investigate the effect of annealing time and experimental conditions on the evolution of the calorimetric glass transition.

9:45 AM

Transforming Powder Processibility by Particle Surface Engineering: *Calvin Sun*[1]; [1]University of Minnesota

The manufacturing of pharmaceutical dosage forms is frequently challenged with deficiencies in physico-mechanical properties of constituting molecular solids. There is a pressing need to replace the empirical formulation and process development with scientifically rigorous design and engineering based on a thorough understanding of relevant material properties and processes, a practice frequently termed as quality-by-design (QbD). We will discuss potentials of the QbD approach in overcoming two common problems in powder processing, i.e., flow and compaction. First, we will show that poor flow properties of fine organic powders can be significantly improved by coating with nano-sized material, which serves as both spacers to reduce powder cohesion and ball bearings to reduce friction. We will then show that polymer coating can profoundly improve compaction properties of fine sand. Fine sand coated with polyvinylpyrrolidone (PVP) exhibits excellent tableting performance because of the formation of a three-dimensional bonding network of PVP upon compaction.

10:05 AM Break

10:25 AM

Multiscale Coarse-Grain Modeling of Nitromethane and RDX: *Sergei Izvekov*[1]; Peter Chung[1]; Betsy Rice[1]; [1]U.S. Army Research Laboratory

A recently developed multiscale coarse-graining (MS-CG) method [Izvekov and Voth, J. Chem. Phys. 123, 134105 (2005); Noid et al., J. Chem. Phys. 128, 244114 (2008)] for obtaining short-ranged coarse-grain (CG) potentials from atomistic level interactions was applied to two conventional energetic materials, nitromethane and cyclotrimethylenetrinitramine (RDX). For nitromethane one-bead and two-bead models fitted to liquid phase simulations at ambient conditions were developed. For RDX, one-bead and four-bead models were derived from crystal and liquid phase simulations to improve transferability of the model across different phases. Performance of resulting models in a simulation of crystal and liquid phases in a broad range of thermodynamic conditions was evaluated against underlying atomistic simulations and experiment. CG models performed reasonably well in a reproduction of various bulk structural and thermodynamic properties, including radial distribution functions,thermal expansion properties, bulk modulus.

10:45 AM

RDX Material Properties Containing Defects: *Lynn Munday*[1]; Peter W. Chung[1]; Betsy Rice[1]; Santiago Solaris[2]; [1]U.S. Army Research Laboratory; [2]University of Maryland

Orientation-dependent material properties of RDX crystals containing defects are explored using molecular dynamics with Smith's (1999) flexible molecular potential. Defects in energetic materials are of interest due to their role in triggering chemical decomposition of molecules through the development of hot spots. The RDX crystal is known to be approximately orthotropic and this work will explore the effect of crystal defects on these orthotropic material properties. General types of defects in RDX are known experimentally and from some predictions in literature. We specifically calculate the defect core structures for single dislocations and limited studies with two sessile dislocations to show the substantial effect of the defect orientation on the melting temperature and shock Hugoniot curve.

11:05 AM Invited

Unraveling Shock-Induced Chemistry Using Ultrafast Lasers: *David Moore*[1]; [1]Los Alamos National Laboratory

The exquisite time synchronicity between shock and diagnostics needed to unravel chemical events occurring in picoseconds has been achieved using a shaped ultrafast laser pulse to both drive the shocks and interrogate the sample via a multiplicity of optical diagnostics. The shaped laser drive pulse can produce well-controlled shock states of sub-ns duration with sub-10 ps risetimes, sufficient for investigation of fast reactions or phase transformations in a thin layer with picosecond time resolution. The shock state is characterized using ultrafast dynamic ellipsometry (UDE) in either planar or Gaussian spatial geometries, the latter allowing measurements of the equation of state of materials at a range of stresses in a single laser pulse. Time-resolved processes in materials are being interrogated using UDE, ultrafast infrared absorption, ultrafast UV/visible absorption, and femtosecond stimulated Raman spectroscopy. Recent results will be presented, and future trends outlined.

11:35 AM Invited

Engineering of the Thermo-Mechanical Response of Molecular Crystals by Solid Solution Impurity Control: *Daniel Hooks*[1]; [1]Los Alamos National Laboratory

Crystalline molecular solids are widely used as pharmaceutical ingredients, dyes, foods, optical elements, electronic materials, and explosives. In many classes of materials (e.g. metals) knowledge of phase behavior and structure-property relations of multi-component systems are used to enormous advantage in engineering materials for specific uses. This is not generally the case for molecular materials because structure-property knowledge is sparse for single component systems and almost entirely absent for more complex multi-component systems. The interactions that direct intermolecular assembly are so subtle that interpretation of structure-property relations are founded on hindsight rationalization in all but a few cases. We have recently prepared molecular crystals with engineered solid solution behavior. The resulting materials have different phase behavior and mechanical response. Material preparation and property characterization, including resulting phase diagrams and elastic-plastic response will be discussed. Plans to include engineering of more complex multi-component crystal systems will also be described.

General Poster Session

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS Extraction and Processing Division, TMS Light Metals Division, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division

Program Organizer: Mark Palmer, Kettering University

Mon-Wed PM Room: Exhibit Hall
February 15-17, 2010 Location: Washington State Convention Center

3D Interconnected Calcium Phosphate Scaffolds for Bone-Tissue Engineering: *Mohammad Tarafder*[1]; Shashwat Banerjee[1]; Vamsi Balla[1]; Amit Bandyopadhyay[1]; Susmita Bose[1]; [1]Washington State University

Calcium phosphates (CaP) are widely used in bone tissue engineering due to their compositional similarity with human bone and excellent bioactivity. The objective of the present study is to investigate mechanical and biological properties of calcium phosphate based 3D interconnected biodegradable porous scaffold using 3-D ceramic printing technology, one of the solid free-form fabrication (SFF) methods. SFF method allows to fabricate structures with controlled geometry and architecture. It's a layer by layer manufacturing process in which a 3D ceramic scaffold is printed by printing a chemical binder onto powdered calcium phosphates. 3D interconnected porous scaffolds with pre-set dimension and pore size have been successfully made using 550 nm ß-tricalcium phosphates. Suitable temperature and layer hights have been optimized. Over 87% sintered density was obtained after sintering the scaffold at 1250^{0}C. Different dopants were also added to investigate their effects on the mechanical and biological properties of these scaffolds.

A Materials Investigation of the UV Degradation of Eco-Friendly, Polypropylene Polymer Composites with Kenaf Fibers: *Christine Carpenter*[1]; Katherine Chen[1]; Christina Blattner[1]; Katie Greenstein[1]; Robert Arens[1]; Edmund Saliklis[1]; [1]Cal Poly State University

Eco-friendly composites of recycled polymers and agricultural waste fibers have been developed for commercial markets, and are currently being pursued as thin shell, curvilinear architectural structures and emergency shelters. However, better understanding of the mechanical properties and the degradation mechanisms are imperative for the development of these materials. This study concentrates on polypropylene (PP) homopolymer and co-polymer composites with kenaf fibers. The effect of accelerated weathering was conducted with ultraviolet (UV) radiation (300-350 nm) and humidity to simulate outdoor conditions. Up to 2000 hours of exposure was conducted, and samples were characterized at every 500 hour interval. Tensile tests and four-point bend tests were conducted, and the stiffness of the composites was found to decrease over time, but the homopolymer and copolymer composites had different behaviors. Fourier-Transformed Infrared Sprectroscopy (FTIR) revealed that the fibers break down and the cellulose-polypropylene bond weakens as a result of irradiation and moisture cycling.

A Molecular Dynamics Study of the Tensile Deformation Behavior of Au Nanowires: *Na-Young Park*[1]; Ho-Seok Nam[1]; Pil-Ryung Cha[1]; Seung-Cheol Lee[2]; [1]Kookmin University; [2]Korea Institute of Science and Technology (KIST)

We performed molecular dynamics simulations for the tensile deformation behavior of Au nanowires. Au nanowires have FCC rhombic structures with a <110>-crystallographic orientation and with four {111} lateral surfaces. In order to investigate the effect of nanowire dimension and different empirical potentials on the deformation behavior, nanowires with the widths ranging from 4nm to 20nm were considered and three different empirical embedded atom method potentials were considered. All nanowires showed the plastic deformation by twin formation and the migration of twin boundaries which induces the formation of <100>-oriented grain along tensile direction and its growth. The yield stress was observed to increase with decreasing nanowire dimension and the change of deformation mechanism was observed between 4nm and 10nm widths. The deformation behavior of nanowires also shows strong dependence on the empirical potentials, which will be also presented in this study.

A Study of the High Rate Response of Squeeze Cast Magnesium Alloy AZ91: Phil Gullett[1]; Wilburn Whittington[1]; Michael Fortier[2]; [1]Mississippi State University; [2]University of Rochester

The uniaxial compressive response of squeeze cast magnesium alloy AZ91 has been measured for material with different cross-section thicknesses. Samples have be tested at strain rates varying from quasi-static to 4000 s-1. The high strain rate tests were performed using a Split-Hopkinson Pressure Bar. Microstructural evaluations were performed before and after testing to correlate the evolution of porosity, grain size distributions, particles size and geometrical distributions, and twin size distributions with mechanical response of the Mg-alloy material.

A Study on the Microstructure and Mechanical Properties of the Powder Injection Molded WC-8%Co: *Sung-Hyun Choi*[1]; Kyoung-Rok Do[1]; Sang-Dae Kang[1]; Kwon-Koo Cho[1]; In-Shup Ahn[1]; [1]Gyeongsang National University

This study was investigated for microstructure and mechanical properties of WC-8%Co alloy system fabricated by PIM process. After WC-8%Co mixed-powder were PIMed, debinding process were carried by 2-steps methods with thermal debinding and solvent extraction. After solvent extraction to eliminate the binder, thermal debinding was examined at the temperature between 250 and 500°C, in the mixed gas atmosphere of N2 and H2. After debinding process, specimens were vacuum-sintered at 1380°C. The transverse rupture strength(TRS) and hardness were measured. The microstructure and phase were observed by XRD, TEM and SEM. In the case of sintered WC-8%Co at 1380°C, the transverse rupture strength of 2000MPa was obtained, and the hardness was 90HRA. The relative density of PIMed WC-8%Co was 99.5%.

A Study on the Microstructures and Electromagnetic Interference Shielding of Sn-Al-Ni Thin Films: Hung Fei-Yi[1]; *Hung Fei-Shuo*[2]; Chiang Che-Ming[2]; Lui Truan-Sheng[3]; [1]Institute of Nanotechnology and Microsystems Engineering, Center for Micro/Nano Science and Technology, National Cheng Kung University; [2]Department of Architecture, National Cheng Kung University; [3]Department of Materials Science and Engineering, National Cheng Kung University

Electromagnetic interference (EMI) is a new form of pollution discovered in recent years. The elements Sn and Al not only possess EMI shield efficiency, but also have acceptable costs. In this study, sputtered Sn-Al thin films with Ni doped (1 wt.%) were used to investigate the effect of the crystallization mechanism and film thickness on the electromagnetic interference (EMI) characteristics. In addition, the annealed microstructure, electrical conductivity and EMI of the Sn-Al films and the Ni-doped Sn-Al films were compared. The results show that Sn-Al film increased the electromagnetic interference (EMI) shielding after annealed. For the Ni-doped Sn-Al films with higher Ni atomic concentration, the low frequency EMI shielding could be improved. After annealing, the Sn-Ni and Al-Ni intermetallic compound (IMC) of thin film distributed in the matrix. This metallurgical effect not only enhanced the diffusion of atoms to the grain boundaries, but also promoted the high frequency EMI shielding.

A Study on the Stress Test of Truck Frames for Freight Trains: *Sung Cheol Yoon*[1]; [1]Korea Railroad Research Institute/Railroad Safety Research and Testing Center

The truck that is used as running equipment for freight train support is a core structural part that supports the load of the car body and that greatly influences the safety of freights and vehicles, as well as their running performance. The running equipment is composed of truck frames, wheels and wheel axles, independent suspensions, and brakes. Among these components, the truck frame supporting the load of the vehicles and freights may be the most important one. This study was carried out to analyze the structure of truck frames and to determine whether they are safe when the maximum vertical load, breaking load, and front and rear loads are applied to them. This was done by subjecting the truck frames to stress tests and then measuring the stress on each of their parts.To measure the stresses based on the results of the structural analysis, strain gages were attached to the surfaces of truck frames. The results of the stress tests showed that truck frames have a safe vehicle load design.

A Study on the Structural Design of the Car Body of a Locomotive: *Sung Cheol Yoon*[1]; Jeongguk Kim[1]; Myung Yong Kim[1]; Kang Youn Choe[1]; [1]Korea Railroad Research Institute/Railroad Safety Research and Testing Center

This study was carried out to analyze the structure of the car body of a locomotive, and to subject such car body to a load test to determine whether it is structurally safe when the maximum load is applied to it. The car body of a locomotive is an important structure that must support the locomotive's under frame, bolster, side frame, roof, and main equipment, including the heavyweight machinery and electric equipment installed inside it. Based on the load conditions in accordance with the enforced "Guide to the Safety Standards in Railway Rolling Stock" in the Railroad Safety Act, a structural analysis and a load test were carried out. The load test was carried out by referring to the results of the structural analysis. The results of the load test showed that the car body of a locomotive has a safe and stable load design.

A Study on the Structure and Mechanical Properties of HSS T42 Steel Using Powder Injection Moulding Method (PIM): *Kyoung-Rok Do*[1]; Sung-Hyun Choi[1]; Sang-Dae Kang[1]; Su-gun Lim[1]; In-Shup Ahn[1]; [1]School of Nano and Advanced Materials Engineering, I-Cube Center, K-MEM R&D Cluster

High speed steels (HSS) were used as cutting tools and wear parts, because of high strength, wear resistance, and hardness together with an appreciable toughness and fatigue resistance. Conventional manufacturing process for production of components with HSS was used by casting. The powder metallurgy techniques were currently developed due to second phase segregation of conventional process. The Powder injection mould method (PIM) was received attention owing to shape without additional processes. The experimental specimens were manufactured using the PIM with T42 powders and polymer. Polymer degradation temperatures were investigated. Specimens were sintered in vacuum and the N2-5%H2 gases atmosphere at between 1150 and 1240°C. Density and Hardness measurement were examined. Microstructures were investigated by SEM, XRD and TEM. Polymer degradation temperature about optimum condition was found at 450°C. 8.3g/cm3 density and 55HRC hardness were observed at 1230°C sintering temperature. Carbide microstructures of smaller and well dispersion were observed at 1230°C.

A Thermo-Kinetic Model and Experimental Analysis of Multiple Passes Laser Phase Transformation Hardening by Using High-Power Direct Diode Laser: *Soundarapandian Santhanakrishnan*[1]; Radovan Kovacevic[1]; [1]Southern Methodist University

Laser phase transformation hardening (LPTH) based on rapid heating and cooling cycles produces hard and wear-resistant layers at the metallic component. However, a tempered zone is formed in overlapped regions of a large hardened area during multiple passes. This study is focused on the development of a thermo-kinetic model to minimize the softening effect due to tempering by multiple passes. A back tempering model is coupled with the thermal model to predict the hardness distributions across the multiple passes hardened area. A tool steel AISI S7 is hardened by using different levels of laser power (1200 W- 1800 W) with different scanning speeds (5 mm/s- 25 mm/s). The effect of multiple passes on the formation of tempered martensite is studied for different overlapped configurations (1mm – 3 mm). The thermo-kinetic model is validated with the experimental results to optimize the processing parameters for multiple passes laser hardening.

Aerosol Route Synthesis of Copper Oxide Nanoparticles Using Copper Nitrate Solution: Burcak Ebin[1]; Ovgu Gencer[1]; *Sebahattin Gurmen*[1]; [1]Istanbul Technical University

Copper oxide nanoparticles show unique features such as electronic, optical, thermal and magnetic properties depending on particle dimension and high surface to volume ratio. Applications of copper oxide nanoparticles cover a large field from gas sensors to magnetic storage media, solar energy transformation to semiconductors and catalysis. We report preparation of the copper oxide nanoparticles by thermal decomposition of the copper (II) nitrate (Cu(NO3)2.3H2O) based aerosol droplets. We studied the effects of reaction temperature on size, morphology and crystallinity of copper oxide nanoparticles under air atmosphere. Scanning Electron Microscopy (SEM) analyses revealed that nearly 30 nm sized copper oxide spherical nanoparticles were synthesized. Energy Dispersive Spectrometry (EDS) analysis show that the weight ratios of Cu to O are 79.89:20.11 for the all samples which are the same ratio with tenorite. Also, X-ray diffraction (XRD) patterns indicate that obtained nanoparticles have monoclinic crystal structure.

AlGaAs-Based Optical Device Fabricated on Si Substrate Using Microchannel Epitaxy: Shigeya Naritsuka[1]; *Daisuke Kanbayashi*[1]; Takuya Kawakami[1]; Yuhei Ando[1]; Takahiro Maruyama[1]; [1]Meijo University

Optoelectronic integrated circuits (OEIC) are very promising to meet an increasing demand for high speed and high capable information processing in telecommunication and computer applications. To realize OEIC, it is mandatorily important to grow dislocation-free GaAs layers on Si substrates. Microchannel epitaxy (MCE) is known as an excellent way to reduce both dislocation density and residual stress in heteroepitaxy [1]. In this paper, AlGaAs-based resonant cavity light emitting diodes (RCLED) are fabricated on the dislocation-free GaAs areas grown on Si substrates using MCE. These LEDs show superior characteristics as good as those fabricated on GaAs substrates. It is also found from a preliminary life test that the LEDs operate more than 300 hours without any degradation. [1] Y. Ujiie, T. Nishinaga, Jpn. J. Appl. Phys, 28 (1989) L337. This work was partly supported by a Grant-in-Aid for Scientific Research on Priority Areas (B) No.18360155 from MEXT in Japan.

Ambient Temperature Stress Corrosion Cracking of 304L Stainless Steel: *Swati Ghosh*[1]; Vivekanand Kain[1]; [1]BARC

Effect of plastic deformation induced by cold rolling or surface machining on the susceptibility to Cl-SCC at ambient temperature of 304L SS was investigated in this study. The as received material was (a) solution annealed, (b) cold worked (CW) and (c) surface machined to induce different levels of strain/stresses in the material. Subsequently constant strained samples were produced for each condition and these were exposed to 1M HCl at ambient temperature until cracking occurred. Subsequently the cracked samples were characterized in detail using stereo microscopy, optical microscopy,atomic force microscopy and EBSD.The results obtained highlight for the first time the effect of microstructural changes produced by straining on the mechanism of crack initiation and propagation at ambient temperatureon in chloride environment.

Anisotropic Behavior of Rolled AZ31 Magnesium under Quasi-Static and High Rate Loading: *Phil Gullett*[1]; Matthew Tucker[1]; [1]Mississippi State University

The anisotropic mechanical response of rolled magnesium AZ31B was examined for quasi-static and high rate loading conditions. Strong strain rate dependencies were observed in the compressive yield, hardening rate, ductility and toughness in the normal direction while rate dependence in the rolling and transverse directions was limited to the hardening response. Therefore, the material texture played a significant role in the mechanical response at both quasi-static and high strain rates. In-situ thermal measurements and micro-structural evaluations (grain size distributions, particles size and geometrical distributions, and twin size distributions) are correlated to the mechanical response.

Analysis of Oxide Formation in High Mn Twinning-Induced Plasticity-Aided Steel during Dew-Point Control: Woong-Pyo Hong[1]; Sung-Il Baik[1]; *Sung-Dae Kim*[1]; Gyo-Sung Kim[2]; Sun-Ho Jeon[2]; Kwang Geun Chin[2]; Chang-Seok Oh[3]; Young-Woon Kim[1]; [1]Seoul National University; [2]POSCO Technical Research Laboratory; [3]Korea Institute of Materials Science

To improve a wettability of molten Zn in Twin-Induced Plasticity(TWIP)-aided steel, it is necessary to minimize the surface Mn-oxide, which is controlled by dew-point (DP) control. In this study, oxides formations under different DP controlled environment were investigated at the surface of TWIP steel. DP temperatures were changed from 0°C to -60°C in the gas mixture of H2/N2 ratio of 15:85 in volume. Morphologies and the distributions of the Mn-O oxides will be reported from the results of cross-sectional view in scanning transmission electron microscopy. Mn depletion regions were observed with the DP above -20°C and the distribution of the surface oxide dramatically changed in the DP temperature range between -20 and -40°C. Ferrite structures were found in the Mn-depleted region near the surface. Surface and internal oxidation revealed that the fast diffusion path along the grain boundaries of ferrite.

Annealing Behavior of TiO2-Sheathed Ga2O3 Nanowires: *Chongmu Lee*[1]; Hyunsoo Kim[1]; Changhyun Jin[1]; Jina Jun[1]; Chanseok Hong[1]; Jungwoo Kang[1]; [1]Inha University

Ga2O3-core/TiO2-shell nanowires have been synthesized by a two step process: thermal evaporation of GaN powder on Au-coated Si substrates and sputter-deposition of TiO2. Transmission electron microscopy and X-ray diffraction analysis results reveal that the Ga2O3 cores and the TiO2 shells are crystalline with monoclinic and tetragonal structures, respectively. Photoluminescence measurements show a red emission peak centered at around 700 nm. Our results also show that coating Ga2O3 nanowires with thin TiO2 layers can significantly enhance the red emission intensity. The PL peak intensity of the Ga2O3/TiO2 coaxial nanowires prepared by sputter-deposition of TiO2 for 1.5 min on Ga2O3 nanowires and then annealing is about 20 times as high as that of Ga2O3 nanowires. X-ray Photoemission spectrometry analysis results suggest that the PL enhancement is attributed to increases in the concentrations of deep levels such as oxygen and titanium interstitials as well as the density of interface states.

Atomic-Scale Characterization of Grain Boundary Embrittlement in Structural Steels: *NamSuk Lim*[1]; JaeBok Seol[1]; ChanGyung Park[1]; Raghavan Ayer[2]; Howie Jin[2]; Russell Mueller[2]; [1]Pohang University of Science & Technology; [2]ExxonMobil Research & Engineering

Intergranular embrittlement of structural steels is characterized by lower impact toughness and is caused by exposure of the steel in the susceptible temperature range, typically around 400°C. This phenomenon is postulated to be associated with preferential grain boundary segregation of solute elements (e.g., S, P). However, direct measurement of atomic segregation has not been possible due to the limitations in characterization methodologies in both spatial and mass resolution. Advances in high-resolution characterization techniques would enable reliable determination of the grain boundary chemistry at near atomic spatial resolution. The present study was performed determine the grain boundary chemistry in quenched and tempered 4340 steels by Atom Probe Tomography. The presentation will describe the methology developed to prepare site-specific specimens and characterization results on the grain boundary composition in steels in the as-quenched and quenched and tempered at 400°C.

Atomistic Study of Dislocation/Vacancy Interactions in bcc Metals: *Zhiming Chen*[1]; Matous Mrovec[2]; Peter Gumbsch[1]; [1]Institut für Zuverlässigkeit von Bauteilen und Systemen, Universität Karlsruhe (TH); [2]Fraunhofer-Institute Für Werkstoffmechanik

In the present work we investigate the interaction of ½<111> and <100> dislocations with a vacancy in body-centered cubic (bcc) metals tungsten and iron by means of atomistic simulations. Two models with a different level of sophistication have been employed for the description of interatomic interactions -- the empirical Finnis-Sinclair potential, which is a central-force scheme, and the bond-order potential, which is based on the tight-binding theory and is therefore able to describe correctly directional covalent bonds that are crucial for the cohesion and structure of bcc transition metals. In order to study the influence of the vacancy on dislocation mobility, the nudged elastic band method was employed to determine the changes of the energy barrier for the dislocation motion. Our simulations show that the dislocation mobility may be strongly influenced by the presence of vacancies and that the change of the energy barrier depends sensitively on the vacancy position.

Basic Study on Synthesis of Sphalerite with Low Iron and Oxygen Pressure Acid Leaching of Sphalerite: *Yan Gu*[1]; Ting-an Zhang[1]; Gouzhi Lv[1]; Zhihe Dou[1]; Yan Liu[1]; Weiguang Zhang[1]; [1]Northeasten University

Pressure leaching performance of sphalerite was studied using synthesized spalerite containing low concentration iron as raw material. The zinc element entering into leaching solution as ions and the sulfur entering into slag as elementary substance. Effects of process parameters on leaching rate of sphalerite and conversion rate of sulfur were researched. Results show that the reasonable parameters are particle size -260 mesh, stirring speed 500 rad/min, leaching temperature 150 °C, oxygen partial pressure intensity 1.0 MPa, initial sulfuric acid concentration 150 g/l, leaching time 90 min, solid-liquid ratio 10:1 (ml:g). The leaching rate of the zinc, iron and sulfur can reach above 95%, 33.5% and 65% at this condition. The kinetic study of pressure leaching was studied. Results show that as to zinc leaching process is controlled by surface chemical reaction and follows kinetic law of "shrinking of unreacted core model", and its reaction activation energy is 73.58 kJ/mol.

Carpenter ACUBE™ 100 an Alternative Copper-Beryllium Alloy for High-Load Bushings and Bearings Applications: Rick Frank[1]; *Karl Heck*[1]; Joseph Stravinskas[1]; [1]Carpenter Technology

Carpenter ACUBE™ 100 alloy is a non-magnetic, cobalt-based alloy exhibiting high strength, excellent corrosion resistance, and outstanding wear resistance. Exposure to beryllium dust has been tied to a variety of health hazards. ACUBE 100 is beryllium free, eliminating the health and safety issues associated with beryllium-containing alloys. The ACUBE 100 alloy can be considered as a direct replacement for copper-beryllium alloy to the AMS 4533 specification.Made by premium-melting and processing operations, ACUBE 100 has demonstrated excellent corrosion resistance to salt spray, nitric acid, acetic acid and humidity. Processing by warm working (work strengthen condition) produces a yield strength of 140 ksi (965 MPa) for use in applications which require superior resistance to galling and wear such as bushings, bearings and other rotating parts that are exposed to corrosive environments and/or subject to high stress and heavy loads.

Cations Removal from Synthetic Neutral Zinc Leach Solution Using Synthetic Iron Oxide: *Mamata Mohapatra*[1]; P. Singh[2]; S. Anand[1]; B.K. Mishra[1]; [1]Institute of Minerals and Materials Technology; [2]Murdoch University

Selective separation of heavy metal ions from industrial and waste aqueous solutions is frequently required in hydrometallurgical processing. In recent years many researcher have worked on supported liquid membrane and floatation technique for the removal of Cd(II) from zinc electrolyte solutions. The selectivity of cationic surfactants for anions has been established in several ion flotation experiments including chloride and cyanide metal complexes of Zn(II), Cd(II), Hg(II), and Au(III) investigated foam separation of Cd(II) ions by dodecyl sulfate from aqueous solutions in the presence of electrolytes and found a negative influence of these electrolytes on Cd(II) foam separation. Study of Cd(II) over Zn(II) ions separation in the presence of inorganic ligands by anionic and cationic collectors was also reported. However, no work has been reported on removal of impurities from zinc neutral leach solutions using solid adsorbents. In the present chapter, a synthetic solution of zinc neutral leach (matching with industrial composition) was prepared and the synthetic solid iron oxide/hydroxide samples were used as adsorbents to remove cations from the synthetic solutions. The mixed iron oxide sample was found to be good for Cd(II) removal from neutral leach solution whereas 6-line ferrihydrite and goethite samples showed good adsorption property for nickel and iron removal. A combination of mixed iron oxide and 6-line ferrihydrite/goethite the neutral leach solution can be used for purification of input to zinc electro-winning.

Comparative Study of Microstructural Characteristics of PM Sintering and Plasma Spraying Coating on a Steel Surface: *Zhang Jie*[1]; WANG Maocai[2]; ZHAI Yuchun[1]; [1]Northeastern University; [2]State Key Laboratory for Corrosion and Protection, Institute of Metal Research, Chinese Academy of Sciences

In this paper, a comparative study has been made between microstructural characteristics in coatings prepared by PM sintering and air plasma spray technique. Some interesting results have been achieved. Firstly, wear-resistant coatings can be commonly achieved by these two techniques. Secondly, microstructural morphologies of these two coatings are obviously different, fully dense structure prevails in the PM sintering coating while bedded grain defective structure in the air plasma spray coatings. Thirdly, PM coating possesses finer, much thicker and more homogeneous microstructure than air plasma spray coating.

Comparison of Stress Corrosion Cracking and Hydrogen Embrittlement Resistance of High Strength Aerospace Alloys: *David Wert*[1]; Thomas Werley[1]; [1]Carpenter Technology Corp.

Historically, stress corrosion cracking and hydrogen embrittlement issues with aerospace high strength structural alloys have been addressed by plating parts using cadmium, chromium, or combinations thereof. However, these surface treatments are not 100% effective, and their application and the disposal of the required plating baths often result in environmental issues. For that reason, new grades have been introduced which can minimize or eliminate the use of these protective surface treatments. This presentation will compare recent results of stress corrosion cracking (KI_{SCC}) and hydrogen embrittlement (KI_{HE}) testing of 300M, Custom 465® Stainless, Carpenter Ferrium® S53, and Carpenter AerMet® 100 alloys. These results were generated using the RSL™ Rising Step Load Bend Testing System. The data to be presented represents samples held at potentials ranging from open circuit, where the test sample is freely corroding in 3.5% NaCl test solution, to -1.10 V_{sce}, simulating cathodic charging while being galvanically coupled to zinc.

Corrosion Behavior of Al-Si-Cr-Ni-Cu Bearing Low Carbon Steel in a Cyclic Dry/Wet Laboratory Test: *Dongping Zhan*[1]; Huishu Zhang[1]; Songlian Bai[1]; Zhouhua Jiang[1]; [1]Northeastern University

The corrosion behaviors of two designed low carbon steels which bearing of Al-Si-Cr-Ni-Cu elements and Q235 were tested in a cyclic dry/wet environment containing 0.01mol/L NaHSO3. Rust layers were observed by optical microscope (OM), scanning electron microscopy (SEM) and XRD. The electrochemical behaviors of the steels were studied on the polarization curves and electrochemical impedance spectroscopy (EIS). The results indicate that the mechanical properties and the corrosion-resistant performances of the designed steel are better than those of Q235. The annual corrosion rates of the designed steels reduce 41.2 % than Q235 at least. There are the enrichments of Cu, Cr, Si and Al in the rust layer close to the matrix, which make the rust layer be more compact and protected. The corrosion currents of the two designed steels are lower than that of Q235, the corrosion potentials and rust layer impedances are higher than that of Q235.

Corrosion Behavior of Aluminum Matrix Composite (AMCS) Prepared by Atomization: *Muna Abbass*[1]; Mohammad Waheed[1]; Ali Faris[1]; [1]University of Technology, Baghdad

In this study, metal matrix composite of an aluminum alloy 7020 reinforced by Al2O3 particles with weight percentages of 5%, 7%, and 10% and its size of (53-75) µm were prepared using molten metal atomization technique. Corrosion behavior of aluminum matrix composite (AMC's) in 3.5% NaCl solution was examined using potentiodynamic polarization measurements. The corrosion rate was found to increase as the temperature was nominally raised from 30°C to 38°C and 45°C for the 10%wt of alumina in atomized AMCS samples in 3.5% NaCl solution. At a temperature of 30°C the corrosion rate was found to rise with increasing percentages of Al2O3 particles for the given atomized samples. This is due to galvanic corrosion between the matrix and reinforcement and the presence of second phases around Al2O3 particles in microstructure of AMCS.

Cracking near a Hole on a Heat Resistant Alloy Subjected to Thermo-Mechanical Cycling: Feng-Xun Li[1]; *Ki-Ju Kang*[1]; [1]Chonnam National University

In a hot section of gas turbine, the turbine blades were protected from high temperature by not only a thermal barrier coating (TBC) but also cooling air fed through internal passages within the blade. The cooling air is then passed through discrete holes in the blade surface, creating a film of cooling air, further protects the surface from the hot mainstream flow. The holes are subjected to stresses due to the lateral growth of the thermally-grown oxide, the thermal expansion misfit between the constituent layers and centrifugal force by high speed revolution, which often results in cracking. In this work, the deformation and cracks occurring near a hole on a heat-resistant alloy subject to thermo-mechanical cycling were investigated. The experiments showed that during thermo-mechanical cycling the cracks occur around the hole depending applied stress level and number of cycles, which could be explained by analytic solution.

Defect Energetics and Fission Product Transport in ZrC: *Sungtae Kim*[1]; Young Ki Yang[1]; Tyler Gerczak[1]; Todd Allen[1]; Dane Morgan[1]; Izabela Szlufarska[1]; [1]University of Wisconsin - Madison

ZrC is being considered as replacement fission product barrier and structural layer to SiC in TRistructural-ISOtopic nuclear fuel. Though the formation and evolution of point defects under irradiation is a major mechanism for degradation in nuclear materials, defect properties of ZrC are largely unknown. Therefore, we have determined the point defect energetics in ZrC using ab initio calculations. The C vacancy and C interstitial defects are shown to be energetically favored over Zr vacancies and interstitials, consistent with the formation of C Frenkel defects under irradiation and the C poor ZrC_x (x<1) stoichiometry measured experimentally. To understand fission product retention from ZrC TRISO fuel particles, the Ag diffusion coefficients in ZrC are experimentally measured. This work was performed as part of the Deep Burn Project: Transuranic High-Temperature Reactor Fuel Qualification under a subcontract with the Battelle Energy Alliance.

Deformation Field and Microstructure of Copper in Flat Punch Indentation: *Matthew Hudspeth*[1]; T. Murthy[1]; C. Saldana[1]; Srinivasan Chandrasekar[1]; [1]Purdue University

A study has been made of the deformation field in plane strain indentation of OFHC copper with a flat punch. Deformation parameters displacement, velocity, strain rate and strain are estimated in situ from optical images of the indentation by tracking the motion of asperities on the surface of the copper. The measurements have confirmed the presence of a dead metalzone underneath the indenter and have demonstrated the formation and evolution of regions of intense strain rate (e.g. shear banding), consistent with classical indentation theory. Metallographic studies of the regions surrounding the indentation zone have been made by optical and transmission electron microscopy, as well as through nano-indentation. The resulting post-deformation microstructure and its correlation to the measured deformation parameters is studied.

Deformation in Shock-Loaded Materials: *Veronica Livescu*[1]; John Bingert[1]; George Gray III[1]; Davis Tonks[1]; [1]Los Alamos National Laboratory

Understanding the deformation of materials during dynamic loading remains difficult. A material shock-loaded by high-explosive detonation experiences a complex loading path evolving both spatially and temporally, which implies an evolving balance of hydrostatic and deviatoric stresses. Twinning may be a favored deformation mechanism under shock loading conditions and plays an important role in damage nucleation. This work brings experimental evidence on the progression of deformation in shock-loaded materials to inform and constrain future numerical damage models. Results from Electron Backscatter Diffraction (EBSD) analysis and fracture surface measurements will be discussed in relation to deformation and damage nucleation. Aspects of shock obliquity and microstructural interactions during deformation will be presented and the results of quantification of twin density gradients with respect to distance from the detonation point will be discussed.

Deformation of High Purity Copper Specimens in Compression between Flat and Grooved Dies: *Bashir Raddad*[1]; Teahert Al-hashani[2]; Mohieldeen Abdel-Rahman[3]; [1]El-Fateh University; [2]Academy of Graduate Studies - School of Applied Sciences and Engineering Department; [3]Minia University

Experiments were carried out to generate data on cold compression of high purity copper specimens having different height-to-diameter (Ho/Do) ratios (0.5 to 1.5) between two flat dies having various degrees of surface condition (knurled, dry and lubricated) and between grooved dies having different groove numbers (1 to 3). Different Ho/Do ratios, die surface conditions and number of grooved resulted in different loading characteristics and also different modes of deformation. The latter case resulted forward and backward extrusion modes plus the radial flow resulting from ordinary compression. Three shapes of deformed specimen were obtained according to the number of grooves. Load values decreased as Ho/Do increased and friction condition improved. For a fixed load, displacement increased for higher Ho/Do ratio. For a fixed displacement, however, load level decreased as Ho/Do increased. Surface strains were apparently affected by the above variables.

Dendrite Tip Shape in Pivalic Acid-Ethanol and Succinonitrile-Salol Systems: *Myung-Jin Suk*[1]; Young-Min Park[1]; Young-Do Kim[2]; [1]Kangwon National University; [2]Hanyang University

In the present work, dendrite tip shapes are fitted by parabolic function, and the difference of dendrite tip shapes between the pivalic acid(PVA)-ethanol(Eth) and succinonitrile(SCN)-salol systems which are characterized by anisotropic and isotropic solid-liquid interfacial property, respectively, is quantitatively treated using shape parameters. PVA-Eth system shows slightly higher Z/R value than SCN-salol system, their Z/R values lying in the range 2-4. (Z is the distance from the tip beyond which the parabolic fit starts to deviate from the profile, and R the tip radius.) λp is the distance from the tip beyond which side branching starts to appear, and is different for both sides of the 2-dimensional dendrite profile. The difference of λp between both sides of the dendrite is larger for PVA-Eth system than for SCN-salol, implying that the dendrite of PVA-Eth is more nonaxisymmetric than that of SCN-salol.

Development of In-Situ Mg-Based Bulk Metallic Glass Composites with High Plasticity: *Ka Ram Lim*[1]; Eun Soo Park[2]; Won Tae Kim[3]; Do Hyang Kim[1]; [1]Yonsei University; [2]Seoul National University; [3]Cheongju University

Among main engineering metallic alloys, Mg metal has advantages of the lowest specific weight, a large amount of deposits on the earth and its easy recycling ability for the saving of energy and other natural resources. Therefore, high-strength and high-ductility Mg-based alloys have been under intense investigation. Mg-based bulk metallic glasses (BMGs) were found to have good castability as well as high strength. However, the Mg-based BMGs do not exhibit appreciable plastic deformation. In the present study, Mg-Cu-RE (RE = Gd, Y) alloys with excellent glass forming ability were selected as starting compositions. Mg-based BMG composites were fabricated by addition of a metal element (Al, Ag, Zn). The reinforcing phase embedded in Mg-based BMG matrix hinder the propagation of shear bands, hence retarding the emergence of catastrophic failure in BMG matrix. The details on the mechanical properties and deformation mechanism will be discussed.

Development of Ultrasonic Techniques for Process Control in Iron and Steel Making: *Jagdish Pandey*[1]; Manish Raj[1]; Krishnan Balasubramaniam[1]; Nikhiles Bandyopadhyay[1]; [1]Tata Steel Ltd.

The paper highlights the potential of ultrasonic C scan image analysis system using 5 and 10 MHz focused beam transducers to optimize electromagnetic stirring parameters during continuous casting of steel billets and overall assessment of billet quality including its cleanliness level. The ultrasonic C scan image plot could also reveal columnar and equiaxed grain structure in these billets and the effect of electromagnetic stirring on the change in equiaxed zone could be estimated. This technique also helped in reducing split end and cracking problem during hot rolling of continuously cast billets for thermo mechanically treated steel bars. An attempt was also made to measure viscosity and melting characteristics of mould powder slags used in continuous casting of steel using normal shear wave transducers. The experimental results show the possibility of using such technique for on-line measurement of viscosity and break temperatures of iron making as well as steel making slags/fluxes.

Dissolution of Platinum from Scrap Automotive Catalytic Converters Using a Combination of HCl+H2O2: *Candeniz Uysal*[1]; Serdar Aktas[1]; Eray Kizilaslan[1]; Kelami Sesen[1]; [1]Istanbul Technical University

Dissolution of platinum which is incorporated in automotive catalytic converters is performed through chemical methods. There is a need to develop a cost-effective and environmentally friendly process for platinum dissolution. This poster summarizes research on the possibility of 10 HCl: 1 H2O2 solution to replace aqua regia for the mentioned task. Dissolution of platinum in this solvent was studied as functions of agitation rate, time, liquid/solid mass ratio and the reaction temperature. A comparison of the solvent's efficiency with that of aqua regia was provided at each step. It was demonstrated that 95% dissolution of platinum in catalytic converters could be achieved with 10 HCl: 1 H2O2 solution under moderate experimental conditions, which are easy-to-adopt to the industrial plants.

Dynamics Research on Leaching Process of Bonded Copper Oxides Strengthen by Mechanical Activation: *Liu Wei*[1]; Tang Motang[1]; Tang Zhaobo[1]; He Jing[1]; Yang Shenghai[1]; Yang Jianguang[1]; [1]Central South University

In order to increasing the leaching rate of the bonded copper oxides in the Tang Dan copper mineral of Yunan province of China, the mechanical activation method was used to strengthen the leaching process. The samples were mechanically activated after the free copper oxides were removed. The leaching dynamics research was conducted by leaching the samples unactivated and activated in the system of NH3-NH4Cl-H2O solution. The apparent activation energy of the leaching process of the samples unactivated and activated for 15min and 30min were calculated to be 24.13kJ/mol, 15.40kJ/mol and 14.76kJ/mol, respectively. Granularity distribution and X-ray diffraction analysis indicated that the improving of the leaching effect was the co-contribution of increase of both surface area and imperfection content.

EDM and AWJ Edge Finishing on Surface Morphology of Hybrid Composite Laminates: *Laxminarayana Pappula*[1]; V. Isvilanonda[2]; M. Ramulu[2]; Naga Prasada Rao Boyalapalli[3]; [1]University College of Technology, Osmania University; [2]Department of Mechanical Engineering, University of Washington; [3]Department of Mechanical Engineering, University College of Engineering, Osmania University

Hybrid titanium laminate is the new high strength-light weight material that possesses great potential for high speed and elevated temperature aerospace structural applications. In this research, series of cuts were made on multi-layers hybrid titanium laminates using die sinker electrical discharge machining (EDM) and abrasive waterjet (AWJ) machining processes. It was found that for EDM machining, low power setting resulted in slow cutting rate but smoother surface was achieved. High power EDM cut cause severe melting and rough surface finish. Both EDM conditions generate thermal cracks and heat damages which are detrimental to load bearing capability. AWJ cuts were impressively faster and machined surfaces were relatively smoother than die sinker EDM. Based on extensive optical and scanning microscopic examination of machined surfaces, it is concluded that AWJ is the preferred method to cut hybrid titanium laminate due to faster cut, smaller damage than EDM process.

Effect of Niobium on Solidification Structure of Gray Cast Iron: Zhou Wenbing[1]; Zhu Hongbo[1]; Zheng Dengke[1]; Hua Qin[1]; *Zhai QiJie*[1]; [1]Shanghai University

The effect of niobium on the matrix microstructure has been studied with varied contents of niobium in gray cast iron, and its mechanism is also analyzed. The results show that when the content of niobium is in the range of 0.042~1.48%, the eutectic size is refined, and the lamellar spacing of pearlite is also significantly decreased. Meanwhile, graphite is refined, too.

Effect of Nitrogen Addition on Isothermal Phase Transformation and Mechanical Properties in Biomedical Co-Cr-Mo Alloys: *Shingo Kurosu*[1]; Hiroaki Matsumoto[1]; Akihiko Chiba[1]; [1]Institute for Materials Research, Tohoku University

Effect of nitrogen addition on isothermal phase transformation behavior in a biomedical Co-Cr-Mo alloy without addition of carbon was investigated during aging at temperature between 973 K and 1273 K for up to 90 ks. In the Co-Cr-Mo alloy, phase transformation from fcc to hcp_1 with super-saturation of Cr occurred by massive transformation. With prolonged aging treatment, a lamellar structure consisting of hcp_2 with equilibrium of Cr and σ phases was formed at hcp_1/hcp_1 boundaries by a discontinuous/cellular reaction, expressed by the reaction equation $hcp_1 \longrightarrow hcp_2+\sigma$. The phase transformation is remarkably changed by addition of nitrogen. In the Co-Cr-Mo-N alloy, the phase transformation from fcc to hcp occurs with a significant long incubation period compared with that in Co-Cr-Mo alloy. Besides, lamellar Cr_2N precipitates during phase transformation, suggesting that phase transformation of Co-Cr-Mo-N alloy may be dominant by the eutectoid transformation ($fcc \longrightarrow hcp+Cr_2N$).

Effect of Non-Sinusoidal Oscillation Parameters on Liquid Friction and Lubrication near the Meniscus of Slab Continuous Casting Mold: *Xiangning Meng*[1]; Miaoyong Zhu[1]; [1]Northeastern University

The extremum equation of liquid friction force in meniscus was solved based on momentum and mass conservation, and a mechanism with consideration of shell deformation for flux consumption was presented, then infiltration time and intensity for estimating consumption were proposed, moreover, effect of oscillation parameters on liquid friction, infiltration time and intensity were analyzed. The results show that liquid flux above free surface is periodically infiltrated into gap between oscillating mold and withdrawing slab by negative pressure caused by widening flux channel from last stage of positive strip time until last stage of negative strip time. Flux consumption increases with decrease of oscillation frequency, and friction force is restricted. Improving amplitude is helpful to welding existed surface cracks, but almost has no effect on flux consumption. Non-sinusoidal oscillation factor has an inverse effect on flux consumption and liquid friction respectively, and it should be a constant for invariable casting conditions.

Effect of Particle Size on the Microstructure of Rapidly Solidified Hypereutectic Iron Alloy Powder: *Min Yang*[1]; Yongxiang Dai[1]; Changjiang Song[1]; Qijie Zhai[1]; [1]Shanghai University

Microstructures of atomized hypereutectic iron alloy powders with different diameters were characterized by X-ray diffraction, optical microscopy and scanning electron microscopy. The phase transformation and eutectic colony melting temperatures of powders with different diameters were measured by using differential scanning calorimetry (DSC). The results show that the as-atomized powders are mainly composed of austenite and a composite microstructure of hard (Fe, Cr)7C3 carbide, but, ferrite and a composite microstructure of hard (Fe, Cr)7C3 carbide after annealed. With the increase of the particle size, the phase transformation temperature increases and the eutectic colony melting temperature of powders slightly decreases.

Effect of Silicon Addition on the Microstructure and Mechanical Properties of Extruded Mg-Zn Alloys: *Hwa Chul Jung*[1]; Ji Hoon Hwang[1]; Kwang Seon Shin[1]; [1]Magnesium Technology Innovation Center, Seoul National University

The Mg-Zn alloys have a large age hardening response, stemming from the precipitation of the transition phase (ß'), and consequently offer both good strength and ductility. In the present study, the effect of Si addition was investigated in order to improve room and high temperature mechanical properties of the Mg-6Zn alloy. The precipitation behavior of different phases in the Mg-Zn-Si alloys was examined by thermodynamic simulations using PandatTM software and casting and extrusion experiments. With the addition of Si in Mg-6Zn alloy, the Mg2Si phase, which has a high hardness and melting point, was formed. The morphology of coarse Mg2Si particles observed in the as-cast Mg-Zn-Si alloys was modified by the extrusion process, and the tensile properties of the Mg-Zn-Si alloys were significantly improved. It was also found that the double aging treatment after extrusion and solution heat-treatment significantly increased both the yield and tensile strengths of the Mg-Zn-Si alloys.

Effects of Lamination on Mechanical Behavior of Nano-Structured Aluminum Composite: *Hala Hassan*[1]; Adel El-Shabasy[1]; John Lewandowski[2]; [1]Ain Shams University, Faculty of Engineering; [2]Case Western Reserve University

A nano-structured Al89Gd7Ni3Fe1 alloy was made from extruding its atomized amorphous powder at different extrusion ratios (ER). The effects of changing the notch radius from fatigue pre-crack to 100 µm on mode I fracture toughness were studied at different test temperatures (e.g. 298K and 498K) and the fracture surfaces were studied with SEM [1]. In addition, laminated specimens (nano-structured Al composite/ Al) were fabricated via co-extrusion to investigate the effects of a laminated structure on smooth bend properties as well as notched properties in both the crack arrestor and crack divider orientations. The laminates were either bi-layer or tri-layer laminates. The addition of a ductile layer to the tensile surface of a nano-composite produced higher bend ductility and notched toughness.[1] H. A. Hassan, J.J. Lewandowski, Materials Science and Engineering A, 497 (2008) pp 212-215.

Effects of Material and Process Parameters on Final Residual Stress and Distortion Predictions during Welding of Steel: *Amir Masoud Akbari Pazooki*[1]; [1]TU Delft

It is well known that material properties as well as welding process parameters have a big influence on residual stresses and distortion in welded structures. The main goal of this paper is the analysis of the sensitivity of material properties and process parameters variations on the temperature, stress and strain fields in welding simulations. The properties under investigation are heat conductivity, specific heat capacity, density, Young's modulus, yield strength, thermal expansion, Poisson's ratio, work hardening, process efficiency, heat input and the geometrical parameters of the Goldak heat input model. Two types of steel (DP600 and AISI 316L) are considered. The welding process used in this investigation is Gas Tungsten Arc Welding. All predictions are made by FEM commercial software (Msc.Marc). The final residual stress and distortion in numerical modeling have been validated by experimental measurements such as synchrotron X-Ray diffraction and laser scanning.

Effects of Mesh Size on Final Residual Stress and Distortion Predictions during Welding of DP600 and AISI 316L Steel Plates: *Amir Masoud Akbari Pazooki*[1]; [1]TU Delft

Predictions of residual stress and distortion in welding process are two important topics in welding engineering. FEM is a powerful tool for this reason. Selecting a suitable mesh size can influence the final results in prediction of residual stress and distortion. In this paper the effect of different mesh sizes (Density) on the final predictions of residual stress and distortion of 316L and DP600 steel plates in a GTAW process are presented. The simulation results of stress and distortion have been compared with the results of experiments such as synchrotron X-Ray diffraction and laser scanning.

Effects of Microstructural and Mechanical Length Scales on Fatigue Crack Propagation in Beta-Annealed Ti-6Al-4V: Thomas Villarreal[1]; Ikshawku Atodaria[1]; *Pedro Peralta*[1]; [1]Arizona State University

Effects of grain orientation and crack tip strain fields in relation to applied loading and fatigue crack growth kinetics are studied in beta-annealed Ti-6Al-4V. Electron Backscattering Diffraction (EBSD) was used to characterize Compact-Tension (CT) specimens before and after tension-tension fatigue at constant ΔK, from 10 MPa.m^0.5 to 20 MPa.m^0.5, which result in different plastic zone sizes. In-situ loading and Digital Image Correlation (DIC) are used to obtain crack tip strain fields. Taylor and Schimd factor maps from EBSD data and known slip systems for loading cases approximating crack tip behavior are compared to the measured strain fields to understand local heterogeneities. The strain fields are 'integrated' ahead of the crack tips in order to study relationships among these fields, grain orientation and overall crack growth kinetics, and to elucidate the role of the interaction between microstructural and mechanical length scales in fatigue crack propagation in this material.

Effects of Post-Deformation Annealing Conditions on the Behavior of Lamellar Cementite and the Occurrence of Delamination in High Strength Cold Drawn Pearlitic Steel Wires: Jung Won Lee[1]; *Ui Gu Kang*[1]; Yong Shin Lee[1]; Kyung Tae Park[2]; Wonjong Nam[1]; [1]Kookmin University; [2]Hanbat University

Wire drawing is one of the most effective way to increase the strength. Suspension bridge is generally required to do galvanizing process to avoid corrosion. At this point, The effects of both annealing temperature and time on mechanical properties and the occurrence of delamination in high strength cold drawn pearlitic steel wires were already investigated. For the low temperature annealing, the carbon dissolution into lamellar ferrite due to strain aging which is known for first and second stage of aging would enhance not only the increase of strength but also the occurrence frequency of delamination. Whereas, as annealing temperatures and annealing time increase further, age softening that includes the break-up, spheroidization of lamellar cementite and recovery of lamellar ferrite starts to operate. Consequently, the reduction of carbon content dissolved in lamellar ferrite would result in the decrease of tensile strength and suppress the occurrence of delamination. The voids formed at the surface of globular cementite particle, which were produced during post-deformation annealing at high temperatures for a long time, would act as one of the origins for delamination during torsion test. This paper provides a major cause to explain the occurrence of delamination behaviour of high strength cold drawn pearlitic steel wires.

Effects of Thermal Residual Stress and Whisker Network on Neutron Diffraction Patterns for SiC-Alumina Composites during Creep Deformation: *Juan Kong*[1]; Nikolas Provatas[1]; David Wilkinson[1]; [1]McMaster University

Whisker network deformation inside a creeping matrix must be understood in order to optimize the design of composite materials. Previous modeling suggests that whisker bending is the dominant deformation mechanism in an aligned percolating network. Experiments were done by Quan et al to verify this, using neutron diffraction peak width (FWHM) as a measure of elastic whisker bending, and peak position to monitor average residual thermal stress. These experiments on crept alumina composites containing 20-30vol% of SiC whiskers showed an unexpected decrease of peak width for the <111> whisker peak. In this work, we have used finite element method applied to a representative volume element (RVE) with two types of whisker network to simulate the creep and hot pressing processes: 3-D random-oriented-short-fibre unit cell without contact generated by a random sequential adsorption algorithm; and 2-D regularly aligned percolating unit cells

Effects of Twin on the Mechanical Behavior of Mg Single Crystals: *Hwa Chul Jung*[1]; Ming Zhe Bian[1]; Nam Kyoung Kwon[1]; Kwang Seon Shin[1]; [1]Magnesium Technology Innovation Center, Seoul National University

The mechanical behavior of HCP metals is strongly influenced by their inherent anisotropic characteristics that originate from the crystal structure. The resolved shear stresses that activate the prismatic, pyramidal and <c+a> slip modes are much greater than those required to initiate the basal slip and tensile twin at room temperature. Therefore, the predominant deformation modes of magnesium at room temperature are the basal slip and tensile twin. While the slip behavior of magnesium alloys has been extensively investigated, research on the twin behavior has been rather limited, even though twinning is an important mode of deformation in HCP metals. The interactions between the dislocations and twin boundaries are important because the deformation-induced twins could act as obstacles to dislocation motion. In this study, effects of twin on deformation and recrystallization behavior of Mg single crystals were systematically investigated by scanning electron microscopy and electron backscattering diffraction (EBSD) analysis.

EKOLUBE™, the Economical, Eco-Friendly Solution for Sendzimir™ 20Hi Mills: *Suresh Neelakantan*[1]; Josef Graetz[1]; [1]Magnum Integrated Technologies

Waterbury Farrel™ continues to lead the development of its 20Hi Sendzimir™ mill, with new technologies including As-U-Roll™ Top and Bottom Crown control and advanced 'ZR' housing designs. Now, Waterbury Farrel™ has elevated its ZMill™ technology by designing EKOLUBE™, a new and exciting patented lubrication technology. This new approach to 20 Hi mill lubrication is designed to extend the operating life of backing bearing assemblies, therefore reducing spares, maintenance and downtime costs. As well, it reduces the use of mill lubrication oil consumables, thus significantly reducing mill operating costs. The EKOLUBE™, system is available on the Waterbury Farrel™ 20Hi Sendzimir™ ZMill™, and may be retrofitted to all existing 20Hi Mills. The paper presented at this conference will describe the EKOLUBE™ system, which injects precise amounts of pure lubricant into 20Hi backing bearings from a dedicated hardware and automation system. EKOLUBE®, the economical, Eco-friendly solution for Sendzimir™ 20Hi mills.

Electrical Conductivity Manipulation and Switching Phenomena of PBZT Thin Film by Doping Process: Jiahua Zhu[1]; Sung Park[2]; John Willis[2]; Max Alexander[3]; *John Zhanhu Guo*[1]; [1]Lamar University; [2]NGC Aerospace Systems; [3]Air Force Research Laboratory

Both chemical and physical doping processes were developed to manipulate the electrical conductivity of the (PBZT) in this work. Protonation with hydrochloride and sulfuric acid significantly enhanced the electric conductivity of PBZT thin film and meanwhile switching phenomenon intrigued by an applied voltage was also observed. The mechanisms for the electrical change and the switching phenomena are investigated and explained from the PBZT molecular structure transformation. Reduction with different metals on protonated PBZT increased the electric conductivity significantly. The behind doping mechanism will be discussed. PBZT nanocomposites doped with conductive nanoparticles and other conductive polymers such as polyaniline and polypyrrole for improving electric conductivity were also discussed. FT-IR, XRD, TGA, EDAX and four-point probe testing were used to better understand the mechanism of doping process.

Electrochemical Behavior of Ni-Cr Base Alloys in Corrosive Environment: *Aezeden Mohmaed*[1]; [1]University of Manitoba

The corrosion behavior of two Ni-Cr base alloys is IN600 and IN601 has been evaluated by potentiodynamic polarization in NaCl solution. IN600 has less passivation range in comparison with IN601 is observed. In addition, the passivation current has been found to be higher than that of IN601. Tafel polarization indicates that IN601 is more corrosion resistant than IN600 in different NaCl concentrations.

Electrochemical Behavior of RuO_2-IrO_2-SnO_2/Ti Electrode under Mild and Forced Conditions: *Ozgenur Kahvecioglu*[1]; Servet Timur[1]; [1]Istanbul Technical University

Dimensionally stable anode (DSA®) with a ternary coating of RuO_2-IrO_2-SnO_2 deposited on a Ti substrate was prepared by polymeric precursor (Pechini) method. The nano-structure, morphology and compositions of the coating were characterized by FESEM, XRD and EDS. Chronopotentiometric studies were carried out at two different current densities: 20 mA cm^{-2} (mild condition, MC) and 1000 mA cm^{-2} (forced condition, FC). After each application, linear sweep voltammetry (LSV) and cyclic voltammetry (CV) tests were performed to investigate the electrochemical behavior of the electrode. The FESEM microphotographs showed that columnar based needle like nano-particles occurred on the ridges of the roughened surface whereas more smooth and compact morphology was observed for the flat parts of the surface. It was seen that the electrode maintained its electrocatalytical activity for lower current density region and its stability when an anodic current of 1000 mA cm^{-2} was applied.

Electrochemical Impedance Spectroscopy of SEI on Porous SnO_2/CNT Composite Anode for Lithium Ion Batteries: *Abirami Dhanabalan*[1]; Xifei Li[1]; Yan Yu[2]; Kevin Bechtold[1]; Chunlei Wang[1]; [1]Florida International University; [2]Max Planck Institute for Solid State Research

Tin oxide based composites have been studied extensively because of the high theoretical specific capacity compared to the commercialized carbon anode. During charge and discharge, solid electrolyte interface (SEI) film is formed at the interface between the electrolyte and anode due to the reaction between the anode and the electrolyte. SEI is a thin lithium ion conductive film which protects the anode from co-intercalation of solvents and consequent exfoliation. It has important influence on the irreversible capacity, cycle performance and stability of Li^+ insertion into anode. In this work, impedance studies were carried out on SnO_2/CNT anodes prepared by electrostatic spray deposition (ESD).The deposition temperature and concentration of CNT in the composite were also varied. The electrochemical impedance spectroscopy (EIS) test was performed to understand the formation and the change of SEI film on SnO_2/CNT anode with subsequent cycling. The equivalent circuit was proposed to fit the EIS plots.

Enhanced Mechanical Properties in Mg-Based Ultrafine Eutectic-Dendrite Composites: Jong Youn Lee[1]; Tae Eung Kim[1]; Sung Woo Shon[1]; Won Tae Kim[2]; Do Hyang Kim[1]; [1]Yonsei University; [2]Cheongju University

Nano grained materials exhibit a remarkable improvement in strength when compared with conventional coarse-grained alloys. However these materials generally suffer from insufficient plastic strain and reduced toughness during deformation. In the present study, a possible way to fabricate MgSnZn and MgSnCu nanostructure-dendrite composites with enhanced plasticity has been investigated. Our main focus is to investigate systematically the effect of microstructure evolution on mechanical properties. We prepared in-situ bulk samples with ultrafine scale eutectic-dendrite composite structure via an injection casting method. In particular, alloys with compositions near ternary eutectic composition were investigated to design the microstructure with different length scale. In the case of Mg-Sn-Zn alloys, addition of ~7at% Zn in Mg-10.7at%Sn alloy effectively endows larger plastic strain reaching ~over 10% with a reasonably high strength of ~657MPa.

Enhancing Mineral Beneficiation by High Intensity Power Ultrasound: *Jagdish Pandey*[1]; Manish Raj[1]; Moni Sinha[1]; Nikhiles Bandyopadhyay[1]; [1]TATA STEEL Ltd.

The paper highlights the attempts made at R & D of Tata Steel Ltd. to reduce impurities from iron ore such as alumina, silica and phosphorous under the influence of high intensity power ultrasound using 20 KHz frequency and 220 Watt power. The laboratory trials indicated 5 minutes treatment time for iron ore slurry containing 1:10 solid/liquid ratio could reduce alumina from 1.72 to 1.12 % and silica from 1.70 to 1.34 % whereas no significant reduction in phosphorous was observed. Scanning Electron Microscope (SEM) micrographs revealed the locations on the surface where the alumina phase in the microstructure detached due to ultrasonic treatment for 5 minutes. The possible reason appears to be the cavitation and streaming under the influence of high intensity power ultrasound. Based on the laboratory results, a pilot scale plant to treat 100 Kg of ore/coal has been set up to implement it in the plant.

Evaluation of High Energy Milling Behavior of ZnO Powders in Different Milling Conditions: *Sezen Yakar*[1]; Ahmet Söyler[1]; Burak Özkal[1]; Sebahattin Gürmen[1]; Mustafa Öveçoglu[1]; [1]ITU

In compare to many other techniques, high energy milling is a very effective and simple technique to produce nanocrystalline powders with the possibility of obtaining larger quantities. On the other hand, application of high energy milling is limited because of the contamination problems. In this study, milling behavior of ZnO powder was studied using different equipment including Spex Mixer and planetary ball mill under different milling conditions. Milled powders were characterized via XRD, BET, LPS measurements and SEM observations for the optimization of milling conditions leading nanosized ZnO powders.

Fabrication and Mechanical Properties of NbC-binders (Co, Ni. Fe) Nano-Composite Consolidated by High Frequency Induction Heated Sintering: *Kee-Do Woo*[1]; Duck-soo Kang[1]; Sang-hyuk Kim[1]; Seong-bae Park[1]; Na-young Song[1]; In-jin Shon[1]; [1]Chonbuk National University

Recently, high energy mechanical milling(HEMM) has become a popular method to fabricate nanocrystalline due to its simplicity and relatively inexpensive equipment. Many of the metal carbides (WC, NbC, TiC, etc) are very interesting and important for several industrial applications such as abrasive material, cutting tools, wear resistant parts in wire drawing, extrusion and pressing dies and wear-resistant surfaces. Especially, NbC is a very important material with promising properties such as outstanding hardness, good resistance to chemical attack and excellent electronic conductivity. The aim of this study was to fabricate the nano-sized carbide, NbC based material, with 10vol.%binders(Ni, Co and Fe) by using high frequency induction heated sintering(HFIHS) method. The relative densities of the sintered NbC-10vol.%binders(Ni, Co and Fe) composites by using HFIHS, pressure of 80MPa were respectively about 91.26%, 91.90% and 91.26%. The grain size, fracture toughness and hardness of NbC-10vol.%Co were 33nm, 10.5 MPa•m^1/2 and 1409 kg/mm^2, respectively.

Fabrication of FeS2-Pyrite Cathode by Spray Dryer Methode: *Sang Dae Kang*[1]; Sung Hyun Choi[1]; Kyung Rok Do[1]; Hyo Jun Ahn[1]; In Sup Ahn**[1]; [1]School of Nano and Advanced Materials Engineering, I-Cube Center, K-MEM R&D Cluster, Gyeongsang National University

A lot of studies about the Li/FeS2 secondary battery, which has high ion capacity and energetic density. In order to obtain nano size FeS2 particles, Fe metal salt solution and sulfur solution were prepared for spray drying. Active carbon and iron die-sulfide were mixed with the ratio of 1/3 and 2/3. The mixture was milled in the planetary ball mill to fabricate carbon coated iron die-sulfide particles. The porous compact for electrode was made by sintering the mixture at the temperature range between 400 and 700°. The microstructure was observed by SEM and phase transformation was analyzed by XRD and TEM. The 60 nm size FeS2 particles was obtained by spray drying, and the carbon was coated at the surface on the iron sulfide surface homogeneously, and the relative density of 55% was measured at the electrode compact. The capacity of early charge indicated 900mAh/g and formed.

Fabrication of the Mg/Al Clad Sheet and Its Mechanical Properties: *Beomsoo Shin*[1]; Sockyeon Yoon[1]; Changseong Ha[2]; Seungkwan Yun[2]; Donghyun Bae[1]; [1]Yonsei University; [2]G-Alloy Technology Co., Ltd.

Mg-Zn base alloy cladded with the thin Al1050 sheets were fabricated by means of a hot rolling process at 280°C. Microstructure of the interface and mechanical properties of the clad sheets were investigated. After heat treatment at 230°C for 30 min, average 15 µm sizes of grains were developed in the Mg alloy sheet and Mg-rich layer was found to be developed about 2 µm in thickness at the Mg and Al interface. Tensile test was carried out at the initial strain rate range of 1x10-3s-1 ~ 1x10-4s-1 and the temperature range up to 300°C. The clad sheet shows superior elongation to failure not only at room temperature but also at the elevated temperatures compared to the Mg alloy sheets. During the test, few numbers of cracks which provide the formation of necking are developed in the layer.

Facile Synthesis of Hollow Co3O4 Microspheres by Solution Spray-Oxidation Method and Its Properities as Supercapacitors: *Guo Qiusong*[1]; Du Guangrong[1]; Guo Xueyi[1]; [1]Central South University

The hollow Co3O4 microspheres were synthesized by solution spray-oxidation method. The feed solution was prepared by using CoCl2•6H2O as raw materials, sprayed by using inner mixed air-nozzle and roasted in the erective pipe resistance furnace with compressed oxygen as carrier gas. The as-prepared samples were characterized by FT-IR, XRD and SEM techniques. The results show that the reaction temperature has an important impact on micro-structure and purity during the process of spray and oxidization for cobalt chloride solution, and the hollow Co3O4 microspheres were obtained at 700°. Furthermore, the elcctrochemical tests show that the electrode prepared by the samples exhibits distinct characteristic of capacitance, the electrochemical capacitive properties of the hollow Co3O4 microspheres were evaluated using cyclic voltammetry and alternating current impedance methods. The capacitive properties depict that the sample Co3O4 by spray-oxidation method is capable of exhibiting excellent capacitive performance in 3.0 mol·L-1 KOH electrolytes.

Fast SET Switching Behavior of Nano-Scale AgInSbTe Based Phase Change Memory: *Sung-Hoon Hong*[1]; Byeong-Ju Bae[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. As a phase change material, Ge2Sb2Te5 (GST) material has been mainly used as the phase change material in PRAM cells, however new phase change material should be needed for high density PRAM device because of high operation power. In this study, Ag and In co-doped SbTe based phase change material was used to fabricate phase change memory. It was proved that AgInSbTe material has higher thermal stability than that of GST material by the in-situ measurement of both the temperature dependent X-ray diffraction and sheet resistance. And Fast set speed was proved by measuring a 200nm diameter sized Ag6In5Sb59Te30 nano-pillar phase change device by means of a conducting atomic force microscope (AFM) connected to a pulse generator and voltage source.

Fatigue Life Prediction for Notched Structures Using Mechanistic Multistage Fatigue Model: *Yibin Xue*[1]; Brian Jordon[2]; Mark Horstemeyer[2]; [1]Utah State University; [2]Mississppi State University

Physically motivated mechanistic MultiStage Fatigue (MSF) model is developed to predict fatigue damage state of structural components under variable and multiaxial loading cases. The MSF model depicts the effects of microstructural features on fatigue damage evolution stages, i.e., incubation, small crack growth, and long crack growth. It allows the assessment of variations in fatigue behaviors associated with random microstructural features and stochastic interference between damage progression and microstructural features. The application of MSF model to notch structures under variable loading cases is realized such that variable loads are reorganized at the notch root not only as stress, strain or plastic strain but also as supplementary plastic deformation or residual stresses induced by overloads. The MSF model predicts comparable fatigue lives, and upper and lower bounds of notched structure under variable loading for structural health prognosis of an airframe-wing component under various service conditions.

Fatigue of Hybrid Polymeric Composites on Twisting: *Nikoloz Chikhradze*[1]; Levan Japaridze[2]; Guram Abashidze[2]; Levan Okijava[3]; [1]Mining Institute/ Georgian Technical University; [2]G. Tsulukidze Mining Institute; [3]Zavriev Institute of Building Mechanics and Seismic Stability

In the paper, the results of the testing on twisting of the composites representing an epoxy matrix reinforced by high-strength and high-modulus carbon fiber, basalt and glassy fiber are considered. Reinforcing components were characterized by the following data: linear density of carbon filament 390 tex, of basalt one – 330 tex and of glassy one – 1500 tex. Investigated composites with the corresponding arrangement of each of these reinforcing elements in relation to the product axis is dedicated for the fabrication of the shell and of the spar of wind turbine blade. Composites are prepared by prepreg technology and have the following physical characteristics: density 1,49-1,55 g.cm-2, porosity -9,2-9,7%, phase concentration: of matrix 61,1-67,0%, of fibers 38,9-43,0%. Composites, selected for the testing on twisting differed from the composites of other series by larger values of short-term mechanical strength on tension, compression, bending and shearing.

Finite Element Analysis of Residual Stress of Plasma-Sprayed Coatings on Thick Wall Components Based on Nastran Software: Li-Ping Niu[1]; Ting-an Zhang[1]; Guan-yong Shi[1]; Zhi-he Dou[1]; Ji-cheng He[1]; Xiao-chang Cao[1]; *Dongping Zhan*[1]; [1]Northeastern University

Residual internal stresses of plasma-spraying lies on different materials and technological parameters, it's hard to study by experimental systematic and most of the experimental methods are ruinous, needs to spend a lot of time and funds. In this paper, residual internal stresses were estimated by mathematical analysis based on finite element analysis. Calculated results of the model shows well agreements with the experimental results of Alumina and tungsten coatings on different matrixes (by plasma-sprayed) . The computational results shows that coefficient of thermal expansion, preheating temperature of matrixes and thickness of coating have greater impact on residual internal stressesKey words: plasma-sprayed, residual stresses, mathematical model, finite element analysis

Flip Chip Bonding of Sn-58Bi Solder Bumps Formed on Flexible PCB: *Sehyung Lee*[1]; Yuesoen Shin[1]; Sehoon Yoo[1]; Chang -Woo Lee[1]; [1]Korea Institute of Industrial Technology

Low melting temperature Sn-58Bi solder bumps were formed on the flexible PCB by electrodeposition and joint and reliability properties were evaluated in this study. Diameter of fabricated bumps was 35um. Flip chip bonding was performed under the temperature of 180° and the bonding force of 40 N. Thermal shock test(TS) was performed with the range from -40 to 85°. The IMC growth thicknesses before and after TS test were 2um and 5um, respectively. Shear strengths before and after TS test were 35gf/bump and 20gf/bump, respectively. Shear strength decreased by 40 % after TS compared with that before TS. The mechanism of the microstructural change and bonding strength decrease will be discussed.

Formation of Different Generations of Gamma Prime Precipitates in Rene 88DT Nickel Base Superalloy: *Antariksh Singh*[1]; Junyeon Hwang[1]; Soumya Nag[1]; Srinivasan Rajagopalan[2]; Jaimie Tiley[3]; Gopal Viswanathan[2]; Hamish Fraser[2]; Rajarshi Banerjee[1]; [1]University of North Texas; [2]The Ohio State University; [3]Air Force Research Laboratory

The compositional and microstructural evolution of different generations of γ' precipitates during the continuous cooling, followed by isothermal aging, of a commercial nickel base superalloy, Rene 88DT, have been characterized by three dimensional atom probe tomography (3DAP) coupled with energy-filtered transmission electron microscopy (EFTEM) studies. After solutionizing in the single γ phase field, during continuous cooling at a relatively slow rate (~ 24°C/min), the first generation primary γ' precipitates, forming at relatively higher temperatures, exhibit near-equilibrium compositions, while the smaller scale secondary γ' precipitates, forming at lower temperatures, exhibit non-equilibrium compositions often consisting of excess Co and Cr, while being depleted in Al and Ti content. Subsequent isothermal aging at 760°C, leads to the composition of the secondary γ' precipitates being driven towards equilibrium.

The mechanisms associated with the early stages of nucleation and growth of the different generations of these γ' precipitates will be discussed.

Fracture and Fatigue of Fe-Based Metallic Glass Ribbons: *Adel El-Shabasy*[1]; Hala Hassan[1]; John Lewandowski[2]; [1]Ain Shams University; [2]Case Western Reserve University

Vickers microhardness indentations, tension and notch toughness tests, as well as controlled static and cyclic strain experiments via bending over mandrels of different diameter have been performed on 30 µm thick Fe78Si9B13 metallic glass ribbons. In addition, Fe-Si-Cr-B ribbon used in magnetic applications has also been tested. For the Fe78Si9B13 ribbons Vickers microhardnesses of 910±100 kg/mm2 and 1030±40 kg/mm2 were obtained for the air side and wheel side, respectively. Tensile strengths were 1640±35 MPa. While the notch toughnesses obtained were 94.5±5.5 MPam1/2. The static "bend over mandrel" tests revealed that the ribbons simply deformed via shear banding for mandrel diameters as small as 0.225 mm. Fully reversed flex bending fatigue experiments revealed a fatigue limit of = 260 MPa. SEM examination was used to characterize all fracture surface details.These results are discussed in the light of recent work on metallic glass systems. Funds provided by NSF-EGYPT Collaborative Research Program.

Furnace Pressure Control System: *Robert Voyer*[1]; [1]Hatch

A efficient furnace pressure control is essential in order to achieve fuel efficiency in casthouse furnaces. Some casthouse teams consider present furnace pressure control technology as unsatisfactory and are experimenting with a variety of methods. During this poster session, Hatch will introduce invention for a new, simple and innovative method to be used for furnace pressure control.

Glass Forming Ability and Mechanical Properties of Zr-Based Zr-Al-Ni Metallic Glasses: Yanhui Li[1]; *Wei Zhang*[2]; Chuang Dong[1]; Jianbing Qiang[2]; Akihiro Makino[2]; Akihisa Inoue[3]; [1]School of Materials Science and Engineering, Dalian University of Technology; [2]Institute for Materials Research, Tohoku University; [3]Tohoku University

Recently, bulk metallic glasses (BMGs) with critical diameter more than one centimeter were discovered in Zr-based Zr-Al-Cu and Zr-Al-Co ternary alloy systems. In this study, aiming to develop new Zr-based BMGs with high glass-forming ability (GFA) and good mechanical properties in Zr-Al-Ni system, the thermal stability, GFA, and mechanical properties of the alloys were systematically investigated. The fully glassy samples with critical diameter above 10 mm were obtained in a wide composition range of present system. The BMGs have a large supercooled liquid region (ΔTx) and reduced glass transition temperature (Trg) more than 70 K and 0.54, respectively. Room compression test revealed that the BMGs exhibit a high yielding strength of 1.7~2 GPa and distinct plastic strain. The BMGs also showed good corrosion resistance in 1 N H2SO4 solution. In addition, the crystallization behavior of the alloys was investigated for understanding their high GFA.

Grain Boundary Character Distribution and Mechanical Property of an as Cold Rolled High Nitrogen Austenitic Stainless Steel: Wei Yan[1]; *Yin Shan*[1]; Ke Yang[1]; Wei Wang[1]; [1]Institute of Metal Research

Grain boundary character distribution and mechanical property of a cold rolled stainless steel with high nitrogen content of 0.66% in weight were studied. The employed cold rolling reductions are 0%, 10% and 20%, respectively. It is shown that both yield strength and ultimate tensile strength were almost linearly increasing with increase of the cold rolling reduction, but uniform elongation was decreased. The high nitrogen steel is found to possess the plastic instability stress (PIS), which is independent of cold working condition. The microstructure deformed by cold rolling was studied by transition electron microscopy (TEM). Electron back scattered diffraction (EBSD) was used to further evaluate the evolution of the grain boundary character distribution, which was caused by the planar slipping of dislocations. The combination of the above two characteristics produced a deeper understanding of the relationship between the deformed microstructure and the mechanical property.

Heterogeneous Phase Nucleation and Growth in ß-Ti Alloys: *Robert Williams*[1]; Soumya Nag[2]; Arun Devaraj[2]; Peter Collins[1]; Srinivasan Rajagopalan[1]; Rajarshi Banerjee[2]; Hamish Fraser[1]; [1]The Ohio State University; [2]University of North Texas

ß-Ti alloys exhibit several complex and competing phase transformations, such as the nucleation of the metastable ω-phase at low to intermediate temperatures, ß-phase separation at intermediate temperatures and intragranular nucleation and growth of the α-phase that can be assisted by the ω-phase and/or ß-phase separation. Through study on the commercial Ti-5553 and model Ti-Mo alloy systems, an attempt is made to understand the stability of the ω-phase, and factors governing the nucleation of the α-phase, at low to intermediate temperatures. Using a combination of (HR)STEM, HRTEM, EELS and 3DAP Tomography, the structure and composition of the ω and α phases are investigated for various alloy compositions and thermal histories. Finally, an attempt is made to rationalize ω-assisted a-nucleation and ß-phase separation-mediated nucleation of the α-phase in ß-Ti alloys.

High Reliability Bonding Process Using Ag-Cu Mixed Nanoparticles: *Yoshiaki Morisada*[1]; Toru Nagaoka[1]; Masao Fukusumi[1]; Yukiyasu Kashiwagi[1]; Mari Yamamoto[1]; Masami Nakamoto[1]; Hiroyuki Kakiuchi[2]; Yukio Yoshida[2]; [1]Osaka Municipal Technical Research Institute; [2]Daiken Chemical Co.

Low temperature bonding process using Ag-Cu mixed nanoparticles was investigated. Though Cu nanoparticles is expected to be the material for low temperature bonding, the bonding temperature of ~400° and the bonding pressure of ~20 MPa are need to obtain good joints. In this study, the bonding temperature and pressure were decreased by addition of the Ag nanoparticles and the bonding strength of the joint reached about 50 MPa at the bonding condition of 350° and 10 MPa. Additionally, the sintered layer of the Ag-Cu mixed nanoparticles showed excellent ion migration resistance.

Impact Toughness Enhancement of an Electron Beam Welded Ti-6Al-4V Titanium Alloy through Post-Welding Heat Treatment: *Christophe Buirette*[1]; Julitte Huez[1]; [1]CIRIMAT-ENSIACET

Electron beam welding of Ti-6Al-4V leads to a loss of mechanical properties in the fusion zone such as fatigue or impact toughness. Fast cooling rate and the associated α' martensitic structure are at the origin of this observation. Various parameters of heat treatment, like soaking time above β transus, cooling rates and stress relieving treatment have been investigated. The analysis of the resulting microstructures associated with impact toughness and tensile tests results allows us to point out the efficiency of each post-weld heat treatment. Moreover these different tests are necessary to investigate the fracture toughness of various microstructure, for a better understanding of damage mechanisms.

Impacts of Impurities on the Properties of Secondary Al-Si-Cu Alloys: *Daryoush Emadi*[1]; Musbah Mahfoud[1]; [1]Qatar University

Recycling of aluminum alloys could provide major economic and environmental benefits. In addition to energy savings, increasing the use of recycled metal is also quite important from an ecological standpoint. Therefore, it is essential to identify, develop, and implement technologies that will optimize the benefits of recycling. In recent designs, Al parts have been used in conjunction with other materials, and therefore, tramp or alloying elements from other alloys, such as tin or scandium become trace elements in the recycled Al alloys. The present study discusses the effects of these trace elements on the mechanical properties of secondary 319 alloy in as-cast and heat-treated conditions. Moreover, a new function, Alloy Recycling Index, is discussed as an industry aid to recognizing the relative recyclability of aluminum alloys, with the goal of maximizing the industry contribution to a green environment.

Improvement of Heat Dissipation in High-Power Light-Emitting Diodes Using Highly Heat Conductive Die-Attach Material: *Chia-ju Chen*[1]; [1]National Chung Hsing University

In recent years, applications of high-power light-emitting diodes (HP LED) have constantly increased. HP LED requires high current drives than before and then generates much heat. Only 15~20% of the input power converts to light and the rest converts to heat. The heat generated by LED chip must be dissipated to the environment effectively in order to maintain the thermal stability of the LED devices. In this poster, we proposed a novel composite die-attach material for LED packaging. This composite die-attach material is prepared by adding proper amounts of nanosized diamond particles into commercial Sn-3wt.%Ag-0.5wt.%Cu (SAC305) solder paste. Since diamond is a highly heat conductive material with a excellent heat conductivity of 2300 W/mk, its incorporation into the SAC305 solder paste (~ 20 W/mk) can promote greatly the heat conductive capacity of the die attach materials and thereby dissipates heat more effectively.

In-Plane Compressive Properties of Hybrid Dyneema®/Carbon Fiber Reinforced Polymer Matrix Composites: *Shahram Amini*[1]; John Shaw[1]; Michael Rossol[1]; Frank Zok[1]; [1]University of California, Santa Barbara

The principal objective of the study is to investigate the potential performance benefits derived from the addition of high performance polyethylene fibers to carbon fiber reinforced polymer (CFRP) composites. The study focuses specifically on 3D orthogonal weaves with carbon employed for the warp and weft yarns and Dyneema® for the z-yarns. Experiments on a series of composite panels with various volume fractions of z-yarns demonstrate that the retained in-plane compressive strength following impact is indeed enhanced by the presence of the z-yarns. The benefits derive from a reduced propensity for delamination during impact and buckling of the in-plane fibers during subsequent compressive loading. Analogous trends are obtained for open-hole compression. Insights into the failure mechanisms are gleaned from microstructural examinations of impacted specimens as well as in situ full-field strain measurements during compression testing.

Influence of Cold Working and Grain Size on the Pitting Corrosion Resistance of Ferritic Stainless Steel: *Zhen Li*[1]; Zhouhua Jiang[1]; Huabing Li[1]; Zurui Zhang[1]; [1]Northeastern University

The influence of cold working and grain size on the pitting corrosion resistance of Fe-Cr-Nb-Mo ferritic stainless steel is investigated using optical microscope and electrochemical methods. The pitting corrosion resistance firstly decreases then increases with increasing the cold-rolling reduction. The number of nucleation site of pitting corrosion increases from 0 to 30% cold-rolling reduction which results in the reduction of pitting potential. However, the increment of pitting potential can be attributed to disappearance of grain boundaries, stacked dislocation and uniform microstructure from 40% to 60% cold-rolling reduction. The recrystallization behavior of the steel with 60% cold-rolling reduction occurs completely after 5 minutes annealing time at 1100°. With prolonging the annealing time, the grain size of the steel grows, and the pitting potential of the steel decrease. The smaller grain size promotes the formation of compact passive film and improves the pitting corrosion resistance.

Influence of Forming Ratio on Mechanical Properties of Pipe Line: *Amir Abachi*[1]; Mehdi Naderi[1]; Afshin Erfanfar[1]; Reza Shamloo[1]; [1]Safa Rolling and Pipe Mills Co.

During pipe forming and testing, different layers of plate thickness undergoes in different modes of stress and the competition between the bauschinger effect and strain hardening determines the final properties of the pipe. To investigate the mechanical properties and difference between plate and pipe, tests were carried out on API X52 and X70 line pipe steels. These tests conducted on plate and pipe with different forming ratios. To perform the behavior of plate under different conditions according to forming ratios, a Finite Element simulation used to modeling the response of the material using industrial software based on FEM method. The results show that at a certain forming ratio, the negative difference between plate and pipe properties become positive by elimination of luders elongation.

Influence of Shock Prestraining and Texture on the Dynamic-Tensile-Extrusion of High-Purity Zirconium: *Daniel Martinez*[1]; Carl Trujillo[1]; Joel Montalvo[1]; Victoria Webster[1]; [1]Los Alamos National Laboratory

The mechanical behavior and damage evolution in textured, high-purity zirconium (Zr) is influenced by strain rate, temperature, stress state, grain size, and texture. In particular, texture is known to influence the slip-twinning response of Zr, which directly affects the work hardening behavior at both quasi-static and dynamic strain rates. However, while microstructural and textural evolution of Zr in compression and to relatively low strains in tension has been studied, little is understood about the dynamic, high strain, tensile response of Zr. Here the influence of texture on the dynamic, tensile, mechanical response of high-purity Zr is correlated with the evolution of the substructure. A bullet-shaped sample is impacted into a steel extrusion die using dynamic-tensile-extrusion process. Mechanical Threshold Stress (MTS) modeling will be performed to provide insight into the dynamic extrusion process. Quantitative comparisons between the predicted and measured deformation topologies and extrusion rates will be presented.

Influence of the Magnesium Addition on the Strength, Ductility and Microstructure of Al-7.4Zn At.% Alloy Artificially Aged at Different Times: *J.Baron De la Rosa*[1]; A. García H.[1]; B. Campillo[2]; S. Valdez[2]; [1]FQ-UNAM; [2]UNAM-ICF

Microstructural characterization, tension and microhardness tests were carried out in an Al-7.4Zn at.% alloy in order to know the influence of magnesium content. The microstructure was observed by using scanning electron microscopy, in order to study the phases developed by the aged treatment. The mechanical strength and ductility properties, were investigated by using Vickers microhardness measurements, and tensile test pulled to failure at room temperature using an Instron Universal Testing Machine, at a constant crosshead speed with an initial strain rate of 3 x 10 $^{-3}s^{-1}$ .Microstructure results show the presence of Al_3Mg_2 and $MgZn_2$ on the α-Al matrix for aged samples. In addition, a significant enhancement of the mechanical properties compared to the casting alloy were obtained.

Influences of Rotational Speed and Welding Speed on the Friction Stir Welding between Copper and 304L Stainless Steel: *Yousef Imani*[1]; Mohammad kazem Besharati[1]; Reza Abdi[1]; [1]University of Tehran

Dissimilar friction stir welding between 304L stainless steel and commercially pure copper plates with thicknesses of 3 mm was performed. A number of FSW experiments were carried out to obtain the optimum mechanical properties by adjusting the rotational speed and welding speed in the range of 500-1000 rpm and 14-112 mm/min, respectively and with an adjustable offset of the pin location with respect to the butt line. Microstructural analysis has been done to check the weld quality (defective or defect free). Cross-sectioning of the welds for metallographic analysis in planes perpendicular to the welding direction and parallel to the weld crown was also performed. The mechanical properties of the welds were determined using a combination of conventional hardness and tensile testing. From this investigation it is found that the offset of the pin is an essential factor in producing defect free welds in friction stir welding of copper and steel.

Interfacial Reactions of Pure Sn,Sn-3.0Ag-0.5Cu and Sn-9.0Zn Lead-Free Solders with the Fe-42Ni Substrate: Yu-Ping Hsieh[1]; *Yee-wen Yen*[1]; Chien-Chung Jao[1]; [1]National Taiwan University of Science & Technology

The study investigated the interfacial reactions between Sn, Sn-3.0 wt%Ag-0.5 wt%Cu (SAC) and Sn-9 wt%Zn (SZ) and the Fe-42Ni (Alloy 42) substrate at 240, 255 and 270°. The experimental results indicated that two interneta;llic compounds (IMCs) with different surface morphologies were observed in the Sn/Alloy42 couple. However, both they were the FeSn2 phases. In the SAC/Alloy 42 couples, only the (Fe,Ni)Sn2 phase was formed at the interface. Three layers structure of IMCs were observed in SZ/Alloy 42 couples and they were the (Ni,Fe)5Zn21 phases. Two stages of IMC thickness change were found in three couples. The IMC thickness in these couples increased as increasing reaction times and temperatures, and it was proportional to the square root of reaction time. As the results, the interfacial reaction mechanism of them was diffusion controlled.

Investigation of Possibility to Metallic Interconnector on the IT (Intermediate Temperature) SOFC: Kee-Do Woo[1]; *MinSeok Moon*[1]; Eui-pyo Kwon[1]; Sang-hyuk Kim[1]; Duck-soo Kang[1]; Myeong-han Yoo[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.

Investigation of Weldabiliy during Laser Lap Welding of Dissimilar Al Alloys: *Cheolhee Kim*[1]; Do-Chang Ahn[1]; Namhyun Kang[2]; [1]KITECH; [2]Pusan National University

Requirements in terms of weight reduction in the automotive industry lead to wide usage of aluminum alloys which have low density and good formability. As various kinds of aluminum alloys are applied to the car body structure, the welding technologies between various combinations of Al alloys are also required. The aluminum alloys have high thermal conductivity, high thermal expansion and high affinity for hydrogen so laser welding is one of most preferred joining methods in the automotive industry. This research investigated the overlap welding of dissimilar Al alloy sheets – 5J32 and 6K32. The plates have 1mm thickness, respectively, and a 4kW Yb:YAG disk laser was used as heat source. Al 5J32 and 6K32 have different thermal conductivity and chemical compositions so the arrangement of the plates affected the weld quality of lap welds. The mechanical and metallurgical behaviour of weldment were observed according to the arrangement of the plates.

Investigation on the Compressive Properties and Microstructural of New Sand Polymer Composite: Esmaeil Sadeghi Meresht[1]; Jamshid Aghazadeh[1]; *Mohsen Seifi*[1]; [1]Amirkabir University of Tehran

The development of new construction materials using recycled plastics is important to both the construction and the plastic recycling industries. This work aimed to reuse the PET bottles waste as a partial additive to sand in mortar compositions in form of Sand Polymeric Composite (SPC) so as to reduce the amount of waste and save the environment from its hazards. The resulting products from the PET mortar compositions give comparable performance against compressive strength. Best conditions for the tested variables with weight proportion of sand to PET were 2 at 250c temperature with 5 minutes for stiffing time. The results showed maximum compressive strength around 65 MPa. In addition it was observed from scanning electron microscopy fine microstructure and coherency between filler particles of sand and PET polymeric chain and porosity of structure.

Investigation Surface Faint-Sliver Defects of Cold-Rolling IF Steel Sheets from Slabs Produced by Continuous Casting: *Jian Zhang*[1]; Cheng Dengfu[1]; Li Jianquan[2]; [1]Chongqing University; [2]Vanadium Recovery & Steelmaking Plant, Panzhihua New Steel & Vanadium Co.Ltd

Surface faint-sliver defects of cold-rolling IF steel sheets will have a bad effect on the appearance and use of rolled products. In this paper, it is revealed that Al2O3 is the important reason for causing surface faint-sliver defects of cold-rolling IF steel sheets by detecting the inclusion in the strands and analyzing the quality of finished rolled products. Therefore, some methods can be employed to evidently weaken surface faint-sliver defects of cold-rolling IF steel sheets, which include the ladle slag modifier to decrease oxidizability of the ladle slag, high basicity (CaO/SiO2) refining slag, controlling chemical composition of slag to increase the absorbency of slag to inclusion, improving the clean of steel liquid, decreasing the amount and size of Al2O3 inclusion and properly increasing the heating time of strand in heating-furnace.

Investigations of Shock_Wave Induced SHS Reactions in Ni-Al System: George Oniashvili[1]; Mikheil Chikhradze[1]; Inga Janelidze[1]; *Nikoloz Chikhradze*[2]; [1]Institute of Metallurgy and Materials Science; [2]G. Tsulukidze Mining Institute

Intermetallics, obtained in Ni-Al system are attractive materials for high-temperature structural applications. Synthesis of Ni-Al intermetallics using shock wave compaction technology was the interest of several investigations. The ratio of Ni and Al were selected accordance of phase diagram of Al-Ni. The precursors were processed in ball mill for activation of surfaces before compaction. Particles sizes was 40-80µm. The assembly was placed in explosive container and surrounded with explosive materials. The ammonite, Hexogene were used as explosives. Following SC/SHS compacts were recovered in different shapes and prepared for investigations. Ni-Al powders of two different compositions were explosively loaded in cylindrical mode and successfully realized shock-wave induced reactions. The stress components, generated by pressure impulse, propagated along the surface by constant rate velocity have been theoretically calculated. The SEM and X-ray analyses were carried out for investigation of microstructure and phase composition. The porosity was estimated using the optical microscope.

Joint Strength of Cu-Sn58Bi-Cu Bonding with Cap Bump Thickness Variation: *Yueseon Shin*[1]; Sehyung Lee[1]; Jeonghan Kim[1]; Changwoo Lee[1]; Sehoon Yoo[1]; [1]KITECH/Micro-joining center

Cu pillar bumps has been received great attention in ultra fine pitch 3D packaging. Unlike solder bumps which are collapsed after flip chip bonding, Cu pillar maintained original dimension after bonding, therefore, no bridging occur for ultra fine pitch 3D bonding. In this study, Sn-58Bi on Cu pillar bumps were bonded on the Cu pad and the joint properties were investigated. Sn-58Bi solder were formed onto the Cu pillar bumps with electroplating. The diameters of the bumps were 30 um. Flip chip bonding was performed under the temperature of 180° and the bonding force of 40 N. Shear strength of as-reflowed joint at the cap solder thickness with 5µm was higher than samples with other thickness. In addition, Shear strength decreased with aging time due to IMC growth at the interface.

Kinetics of Titanium and Chromium Carbides Coating Produced on Structural Steel by Thermo-Reactive Deposition Technique: Helal Tahirlu[1]; *Mosaad Sadawy*[1]; Elshan Elshan[1]; Taherli Shirinov[1]; [1]University of Technology

A multi-component diffusion study of titanium and chromium on steel substrate has been studied by pack cementation process. The thickness, structure and hardness of the coated layers have been investigated at different time and temperatures by optical microscopy, X-ray diffraction (XRD) analysis and Vickers micro-hardness tests. The coating layer formed on the steel samples is smooth and compact and well bonded to the steel matrix. The thickness of titanium and chromium carbides layer formed on the steel samples ranged from 20 to 32 µm, depending on temperature and the treatment time. The kinetics of the reaction have also been studied.

Laser Beam Welding of Haynes 188: *Akin Odabasi*[1]; Necip Unlu[1]; Gultekin Goller[1]; Niyazi Eruslu[1]; [1]Istanbul Teknik Universitesi

Haynes 188 (HN-188) is a commonly used Co-Ni-Cr-W superalloy since 1960s (Haynes 188 is a registered trademark of Haynes International, Kokomo, IN, USA). Because of its excellent high temperature strength, good resistance to hot corrosion, and wear resistance, HN-188 has found extensive applications such as afterburner components and combustors. Even the alloy has been investigated previously, new industrial processes such as laser beam applications i.e., laser beam welding, and laser powder deposition, increase the demand on theoretical and experimental knowledge. In this research, laser beam welding characteristics of HN-188 superalloy (2.1 mm thick) were investigated. Two different heat inputs (61.3 J/mm and 90.1 J/mm) and travel speeds (46.5 mm/s and 22.2 mm/s) were applied. The base metal (BM), fusion zone (FZ), heat affected zone (HAZ) and the geometry of weld seams were characterized using optical microscopy (OM) and scanning electron microscopy (SEM). In addition, the welded samples were examined radiographically.

Lattice Constant Effect on the Deformation Behavior of Mg-Zn-Re Alloys: *Sock Yeon Yoon*[1]; Beomsoo Shin[1]; Donghyun Bae[1]; [1]Yonsei University

Since the slip system of the magnesium alloys is significantly limited at room temperature, other deformation modes are imparted during deformation. In this study, we can change the amount of the soluble elements in the matrix by varying the content of the rare-earth in Mg-Zn-Re alloy, thereby developing the alloys having different lattice constants. The alloys are produced under an Argon atmosphere. Lattice parameters are obtained from the X-ray diffraction patterns using the Cohen method. As the amount of the rare-earth element increases, the lattice constants increase in some composition rage. These results induce higher flow stress and enhanced twinability when the lattice constant increases. The deformation behavior of the alloy sheets at room and elevated temperature will be presented.

Local Stress and Strain Analysis of Atomistic Simulations: *Matthew Priddy*[1]; Donald Ward[1]; Phil Gullett[1]; [1]Center for Advanced Vehicular Systems, Mississippi State University

Molecular dynamic simulations are used to examine the failure in isolated triple junctions in aluminum. Understanding the state of the material for which voids nucleate is essential in helping to characterize the conditions that facilitate damage at the nanoscale. The simulations are displacement controlled, uniaxial and biaxial deformation with the voids nucleating at or near the triple junction or along a grain boundary. This work evaluates the local stress, local strain, and local triaxiality to better elucidate the state of the material during deformation. Simulation results for various grain orientations and textures are compared.

Low Temperature Bonding Process Using Cu Nanoparticles: *Toru Nagaoka*[1]; Yoshiaki Morisada[1]; Masao Fukusumi[1]; Yukiyasu Kashiwagi[1]; Mari Yamamoto[1]; Masami Nakamoto[1]; Hiroyuki Kakiuchi[1]; Yukio Yoshida[1]; [1]Osaka Municipal Technical Research Institute

Bonding of oxygen-free copper using various sizes of Cu nanoparticles was investigated. The bonding process was conducted in air under the condition of the pressure of 5-20 MPa and the temperature of 300-400°C. The average sizes of Cu nanoparticles were 7.2 nm, 203 nm, and 498 nm, respectively. The joints with Cu nanoparticles (203 nm) showed the highest shear strength among the samples. Since Cu nanoparticles (7.2 nm) should be coated with Cu_2O before bonding because of its small size, it was difficult to be sintered. On the other hand, it seems that the size of Cu nanoparticles (498 nm) was too large to be sintered at low temperature of 300-400°C. Cu nanoparticles (203 nm) prevented oxidation and showed low-temperature sintering property. Consequently, it seems that the size of Cu nanoparticles (203 nm) should be suitable for low temperature bonding.

Magnetic Properties of High-Coercivity Nanocrystalline Pr-Fe-Co-Al-B Bulk Amorphous: *Lotfi Bessais*[1]; [1]CNRS

The Pr-based bulk-amorphous have attracted much attention as they were regarded as promising magnetic materials. In this study our objective is to improve the hard magnetic properties of the bulk amorphous PrFeCoAlB by a controlled nanocrystallization of the as-milled alloys and understand the nature of the entities responsible for this improvement. Besides magnetic measurements, we have carried out structural investigations, HRTEM , and Mössbauer spectroscopy. PrFeCoAlB bulk amorphous shows a coercivity of 8kOe. The controlled nanocrystallization enhances the coercivity to 30kOe and remanent magnetization to 90emu/g. Those values are the highest ever found for annealed bulk amorphous isotropic systems. The grain size for optimal magnetic properties is around 28nm. The high coercivity is explained by several effects: the exchange coupling F-AF, a low dipolar interaction, and a low value of the effective demagnetizing factor. As a consequence, those systems open a route for promising permanent magnet applications.

Mechanical Properties and Rapid Consolidation of Binderless Nanosturctured Tantalum Carbide from Mechanically Activated Powder by Pulsed Current Activated Sintering: *In-Jin Shon*[1]; Byung-Ryang Kim[1]; Min-Seok Moon[1]; Kee-Do Woo[1]; Na-Ri Kim[1]; [1]Chonbuk University

Industrial applications of metal carbides are cutting tools, hard coating, and hard constituents in the metal matrix composites for high temperature applications because of their great strength, hardness and melting temperature. Among these carbides, tantalum carbide has a very important and promising properties, such as outstanding hardness, high melting point (3880°), good resistance to chemical attack, thermal shock and oxidation, and excellent electronic conductivity. Highly dense nanostructured TaC with a relative density of up to 96% were obtained within 2 minutes by pulsed current activated sintering under a pressure of 80 MPa. The relative density of TaC increased and the average grain size of TaC decreased with milling time. The hardness and fracture toughness of the dense TaC produced by PCAS were 2076, 1645, 1287 kg/mm2 and 6.8, 7.6, 8.9 MPa.m1/2 with milling time for 10, 4, and 1h, respectively.

Mechanical Properties of the Ti-Nb-X%HA Biomaterials Fabricated by High Frequency Induction Heated Sintering Using High Energy Ball Milled Powders: *Kee-Do Woo*[1]; Sang-hyuk Kim[1]; Duck-soo Kang[1]; Jung-nam Woo[1]; Xiaopeng Wang[1]; Zhiguang Liu[2]; [1]Chonbuk National University; [2]Harbin Institute of Technology

Ti and Ti based alloy are widely used as biomaterial due to low density, high strength and good biocompatibility. Especially, Ti-6%Al-4%V ELI alloy is one of the most useful biomaterials. But, Ti-6%Al-4%V ELI alloy has been reported that Al leads to Alzheimer's disease and V is classified into toxic material. Also, Ti-6Al-4V ELI alloy is high elastic modulus material than that of bone. Therefore, biomaterial with low elastic modulus and non-toxic characteristics has to be developed. The aim of this study was to fabricate the Ti-Nb-HA composites by high frequency induction heated sintering (HFIHS) at 1000° under 60MPa pressure using high energy mechanical milled Ti, Nb and HA powders for 0~8hr. After sintering, the physical and mechanical properties of the Ti-Nb-HA composites have been investigated. As results, relative density and hardness of the sintered Ti-42wt%Nb-(0,10,15)wt%HA composites which milled for 8hr were 94%, 611.7kg/mm^2, 95%, 865.2kg/mm^2 ,97% and 882.3kg/mm^2, respectively.

Mechanical Properties of Consolidate of Nanostructured Niti Alloy by Rapid Sintering: *In-Jin Shon*[1]; Na-Ri Kim[1]; In-Yoong Ko[1]; Je-Shin Park[2]; Wonbaek Kim[2]; [1]Chonbuk University; [2]Korea Institute of Geoscience and Mineral Resources

NiTi alloy has been used in many areas such as naval, automobile, robotic, nuclear, aerospace, and biomedical applications because of practical shape memory alloy with high strength, ductility, excellent corrosion resistance, wear resistance, and good biocompatibility. NiTi was synthesized from Ni and Ti powder during the high energy ball milling for 10hours. Dense nanostuctured NiTi was consolidated within 2 minutes from the mechanically alloyed powder by pulse current activated sintering under pressure of 80Mpa. The grain size, hardness and fracture toughness of NiTi sintered by pulse current activated sintering were 166nm, 696kg/mm2 and 7MPa•m1/2, respectively.

Mechanical Strength and Fracture Behavior of Silicon Wafer Based-Solar Cell: *Jai-Won Byeon*[1]; Bong-Kul Shin[1]; Chang-Yong Hyun[1]; [1]Seoul National University of Technology

During mass production of Si wafer-based solar cell, unexpected fractures have been reported to occur at the substrate Si-wafer or thin film layer. Mechanical and thermal stress induced during the fabrication process cause failure at the defects such as microcrack in Si-wafer and interface between substrate and thin film layer. In this study, the effect of saw damages and thickness of Si wafer as well as fabrication process variables on the strength and fracture behavior of solar cell were investigated. Wafers with different thickness from 200 μm to 100 μm were prepared by chemical etching of as-saw wafer. Fracture strength as a function of thickness of Si wafer was measured by four point bending test of over 50 bending specimens in one wafer. Fracture surface was observed to examine crack initiation site by scanning electron microscopy and non-destructive scanning acoustic microscope. These observations were discussed in relation with measured fracture strength.

Mechanical Strength Change of Dissimilar Friction Stir Welded Joint between Al and Mg Alloys by Probe Position Variation: *Yoonki Sa*[1]; Hansur Bang[2]; Heonsun Bang[2]; Yutaka S. Sato[3]; Sehoon Yoo[1]; Changwoo Lee[1]; [1]Korea Institute of Industrial Technology; [2]Chosun University; [3]Tohoku University

Mechanical properties of dissimilar friction stir welding (FSW) joint of Al and Mg alloys were improved by shifting probe position. Significantly high tensile strength of 218.8 MPa, which was 81~87 % of the tensile strength of matrix materials, was achieved when probe position was 0.9 mm shifted toward Al6061 side from the center of the weld. The tensile strength was 182.9 MPa when probe was located at the center and it was 132.3 MPa when the probe was 0.9 mm shifted toward AZ31 from the center. The amount of plastic flow was the highest when probe position was shifted toward Al6061. Finite element analysis indicated that the weld had high and well-distributed temperature on the basis of joint line when the probe position was shifted by 0.9 mm toward Al6061 side. Such thermal characteristics by shifting probe position led to enhance plastic flow and tensile strength.

Microstructural Characterization of the Composite AlZnAg Clad Coating on Alfe: S. Casolco[1]; S. Valdez; [1]ITESM-Puebla

The composite material has been clad by the rolling process. A layer of AlZnAg alloy has been coated on both surfaces by an AlFe film. The characterization was carry out by atomic force microscopy (AFM) and scaning electron microscopy (SEM) in both transversal and longitudinal section zone in order to know the surface morphology. The results show a strong mechanical bond between the AlZnAg and AlFe alloys. In addition the composite-clad material has been deformed by tension test and their results shows bands of strain, due to the superplastic deformation and the small grain size

Microstructural Weak Links for Spall Damage in Polycrystalline Metals: Leda Wayne[1]; *Pedro Peralta*[1]; Darrin Byler[2]; Christine Tomforde[1]; Stephan Digiacomo[1]; Shima Hashemian[1]; Heber D'Armas[3]; Shengnian Luo[2]; Scott Greenfield[2]; Robert Dickerson[2]; Kenneth McClellan[2]; [1]Arizona State University; [2]Los Alamos National Laboratory; [3]Universidad Simon Bolivar

Correlations between spall damage and local microstructure were investigated using multi- and polycrystalline copper samples via laser-driven plate impacts at low pressures (2-6 GPa). The short pressure pulses (250 ns), allowed isolating microstructural effects on spall damage. Velocity interferometry was used to measure free-surface velocity, to monitor spall failure, and to examine changes on the shock response due to microstructure variability. Electron Backscattering Diffraction was used to relate the presence of porosity to microstructural features such as grain boundaries and triple points. Potential sites for preferred damage nucleation and strain localization were identified in terms of their crystallography via statistical sampling in serial sectioned specimens. Results indicate that terminated twins and grain boundaries with misorientations between 25° and 50° are the preferred locations for intergranular damage localization. Two-dimensional hydrocode simulations based on crystallography and geometry of selected damage sites are used to correlate these variables to the presence of damage.

Microstructure and Formation Mechanical of 3D-Meshy SiC/2Cr13 Composite Interface: *Yu Liang*[1]; Ru Hongqiang[1]; [1]Texture of Materials, Ministry of Education, College of Materials and Metallurgy, Northeastern University,

The microstructure, formation mechanism of the matrix and the interface of SiC/2Cr13 composites have been investigated by XRD, EDS attached to SEM. Results showed that the interface included two zones, which are silicon carbide reaction zone(SRZ) and metal reaction zone (MRZ), and the MRZ can be divided two zones, one is the poor chromium zone (PCrZ-MRZ) and the other is rich chromium zone (RCrZ-MRZ). SRZ is mainly composed of the bright matrix of Fe5Si3,Cr7C3,Cr23C6 and Cr3Si, and randomly distributed graphite precipitates. RCrZ-MRZ mainly contains Cr23C6. PCrZ-MRZ is mostly made up of Fe2Si. The order of the interface formation is determined by the solidification rate of the material resultant. Cr23C6 in the PCrZ-MRZ casts firstly. Secondly, Fe2Si casts in the PCrZ-MRZ. Finally, Fe5Si3 deformed by Fe2Si casts in the SRZ. The PCrZ-MRZ hinders the interface reaction by inhibiting the diffusion of Fe atoms from the alloy towards the SRZ.

Microstructure and Mechanical Properties of Al Based Composite Coatings Produced by the Cold Gas Dynamic Spraying Process: *Onur Meydanoglu*[1]; Huseyin Cimenoglu[1]; Eyup Kayali[1]; [1]Istanbul Technical University

In this study, microstructure and mechanical properties (hardness and wear) of Al-B4C composite coatings at various amount of B4C content prepared on structural steel substrate by cold spraying were investigated. Microstructural characterization was performed by XRD, optical and scanning electron microscopes. Hardness values and wear resistances of composite coatings wear measured. It was observed that hardness and wear resistance of composite coatings were higher than that of pure Al coating. Although hardness of coatings increased with increasing amount of B4C content, no significant change was observed in the wear resistances of composite coatings with change of B4C content.

Microstructure and Phase Evolution of Uranium and Dysprosium Nitrides Formed during Reactive Ball Milling: *Brian Jaques*[1]; Daniel Osterberg[1]; Cole Smith[1]; Patrick Callahan[1]; Brian Marx[1]; Darryl Butt[1]; [1]Boise State University

Uranium, dysprosium, and (Ux, Dy1-x) (where X ranges from 0 to 1) metals have been ball milled for different lengths of time in a nitrogen atmosphere. It was found that full conversion of dysprosium metal to DyN occurs in less than 60 minutes and results in a phase pure mononitride, DyN, which has a FCC crystal structure. Ball milling uranium metal in nitrogen results in a phase pure sesquinitride, U2N3, which has a BCC crystal structure. As the uranium content is decreased to 60 mol% the resultant powder is primarily amorphous. However, when the uranium content reaches 50 mol%, a FCC crystal structure is observed. The temperature and pressure of the milling vessel was recorded as a function of time to gain insight into the kinetics of the nitridation reactions. The resultant materials were characterized by means of x-ray diffraction, electron microscopy, and particle size analysis.

Microstructure Changes in Primary Recrystallization of Grain-Oriented Silicon Steel by Pulse Current Intermediate Annealing: *Lihua Liu*[1]; Qiangqiang Xia[1]; Wen Shi[1]; Lijuan Li[1]; Xueliang Wu[1]; Qijie Zhai[1]; Wu Zeng[1]; [1]Shanghai University

The effect of intermediate annealing by pulse current on the grain textures and final magnetic properties of grain-oriented silicon steel sheets produced by one-stage rolling method was investigated. It was found that the texture and microstructure of the sample treated by pulse current are very different from that by conventional annealing treatment. Pulse current annealing, for primary recrystallization, increases the (110) crystal plane to 3 times as strong as that of furnace annealing, and increases the special boundaries with misorientation angles of 20-45°, but has little influence on gain size. Pulse current intermediate annealing improves magnetic properties (B8) and enables to reduce the iron loss in oriented silicon steel after secondary recrystallization. In addition, for pulse current intermediate annealing, from primary to secondary recrystallization Goss texture increased 38 times from primary to secondary recrystallization, for pulse current intermediate annealing but for conventional treatment, only increases 22times.

Microstructure Components and Mechanical Properties of an Acicular Ferrite Pipeline Steel: Wei Wang[1]; *Yin Shan*[2]; Wei Yan[2]; Ke Yang[2]; [1]Electric Power Research Institute, Guangdong Power Grid Corporation; [2]Institute of Metal Research

Through thermo-mechanical controlled processing (TMCP), the acicular ferrite (AF) microstructures with different phase components were obtained in a pipeline steel, and the relation between AF microstructures and mechanical properties was investigated. The results showed that the effective grain size (EGS) reduced obviously with decreasing finish rolling temperature (FRT), but did not change with cooling rate (CR) and simulated coiling temperature (SCT). Lowering FRT or enhancing CR could increase the percentage of granular bainitic ferrite (GF) and bainitic ferrite (BF). The content of high angle grain boundaries (HAGBs) increased with the decrease of FRT when FRT=800°, then decreased with FRT at 750°. It was found that the higher fraction of HAGBs led to the better low temperature toughness. When fine AF was obtained with high GF and BF content and low quasi-polygonal ferrite (QF) content, the steel could possess good strength and toughness.

Microstructure Development of Silicon Steel Prepared by Near-Rapid Solidification: *Xianyong He*[1]; Quanzhi Sun[1]; Lei Wang[1]; Qin Peng[1]; Qijie Zhai[1]; [1]Shanghai University

The aim of this work was to have an insight into microstructure development of silicon steel by thin strip continuous casting. The experiments were designed to approximate the solidification conditions of thin strip continuous casting and carried out under controlled laboratory conditions. The thin strip with three different silicon compositions were prepared by vacuum non consumable arc-melting. Based on the experiments of thin strip casting in lab, the cooling rate was determined by different strip thickness. The effects of compositions on the microstructure of silicon steel thin strip are studied. The results show that the microstructure of thin strip with different composition and thickness are composed of dendrite and equiaxed grain. With change of silicon content and strip thickness, the solidification structure and area percent of equiaxed grain varies significantly.

Microstructures and Four-Point-Bending Fatigue Behavior of Three Kinds of Low-Carbon Steels for Load-Chain Materials: *Wei Wu*[1]; Gongyao Wang[1]; David Huber[2]; Peter Hogan[2]; Rodney Reynolds[2]; Jules Raphael[2]; Peter Liaw[1]; [1]The University of Tennessee; [2]Columbus McKinnon Corporation

Three kinds of low-carbon steels, 10B22, 4615, and 4720, are used in electric hoists as load-chain materials. The microstructures of these low-carbon steels were observed. Four-point-bending-fatigue tests were conducted on cylindrical specimens to examine the fatigue behaviors of these low-carbon steels at different stress levels. The four-point-bending-fatigue tests were performed at a stress ratio of 0.1 and a frequency of 10 Hz with a sinusoidal waveform. The fatigue results showed that the fatigue-strength of the 10B22 steel was the highest at the reference cycles, 107. However, the fatigue-strength of the 4720 steel is the lowest at the same fatigue life. The fractography was investigated by using scanning electron microscopy (SEM), which indicated that the fatigue cracks initiated from the specimen surface and propagated transgranularly.

Microstructures and Mechanical Properties of AM60B-based Eco-Mg Alloys: *Min-Ho Choi*[1]; Dong-In Jang[1]; Shae K. Kim[1]; [1]Korea Institute of Industrial Technology

This paper focuses on the potential to maintain mechanical properties of CaO added Eco-Mg alloys based on AM60B Mg alloy which has been applied to automobile parts where excellent ductility, toughness, and crashworthiness are required. It has already verified that the mechanical properties of CaO addition of below 0.3wt.% as ingredient into AZ31B and AZ91D Mg alloys can be maintained with refined grain size. CaO does not exist as CaO itself in the solidified state. The purpose of this paper is to investigate the tendency of grain refinement and the change of mechanical properties, esp. elongation for CaO added AM60B Mg alloys with respect to CaO contents, on the basis of non-SF6 gas processing and maintaining the alloy's process-abilities. CaO added AM60B Mg alloys were manufactured by conventional melting and casting procedure. Each alloy will be investigated through optical microscope, EDS analysis, and hardness and tensile tests.

Molecular Dynamics Simulation of Au-Rh Precipitates Structure: *Peihua Jing*[1]; Hyon-Jee Lee[2]; Ian Robertson[3]; Jae-Hyeok Shim[4]; Brian Writh[2]; [1]Structural Integrity Associates; [2]Department of Nuclear Engineering, The University of California; [3]Department of Material Science and Engineering; [4]Korea Institute of Science and Technology,

The strength and creep properties of precipitate strengthened materials are controlled by the interactions of dislocations with obstacles, which depend on precipitate coherency, elastic and thermodynamic properties. In this paper, the molecular dynamics simulations of oversized Au precipitates and undersized Rh precipitates are discussed and analyzed as a function of precipitate radius. For Au precipitates,coherency loss is associated with the defected matrix atoms forming an octahedral structure. Dislocation reaction analysis explains the observed structure of a network of Hirth dislocation and Shockley partial dislocations. As the precipitate size increases, additional Shockley partial dislocation loops emanate from the octahedron. For the undersized Rh precipitates, coherency loss involved an octahedral-type structure in the matrix. However, with increasing Rh precipitate size, the coherency loss transitioned to internal precipitate deformation. Evidently, above a critical size, the excess volume associated with an undersized precipitate allows for significant deformation within the precipitate.

Modeling the Effect of the Contact Surface Temperature on the Deformation of an Aluminum Pin During A Wear Test: *Mario Rosenberger*[1]; Elena Forlerer[2]; Carlos Schvezov[1]; [1]Universidad Nacional de Misiones; [2]Comisión Nacional de Energia Atómica

The temperature of the contact surface of aluminum pins increases under dry sliding, the temperature increases the plastic deformation of the subsurface, which moves and places superficial materials on the borders of the pin. A thermal model with asperities on the contact surface was developed to calculate the temperature field of the bulk, which is used in an elasto-plastic model to predict the pin deformation. A three-dimensional model was employed, and temperature dependent mechanical properties were assumed. Loads were applied simulating a test performed in a pin-on-ring machine. A sudden subsurface deformation was observed when the tangential load achieves a well determined value, defined as the critical load. This critical load increases when the temperature diminishes. The results of the model are compared with experiments performed on AA1060 alloys reinforced with 15 % alumina particles. Agreement between predictions and experiments was observed.

Monitoring Particle Pulverization in Composite Silicon Anodes for Lithium Ion Batteries by Acoustic Emission: *Kevin Rhodes*[1]; Claus Daniel[2]; Edgar Lara-Curzio[2]; Nancy Dudney[2]; [1]University of Tennessee; [2]Oak Ridge National Laboratory

Due to the brittle nature of Si, extensive particle fracturing occurs during lithiation which leads to capacity fade and eventual failure of the cell. Better understanding of particle degradation due to cycling is paramount to directing future research aimed to improve this material's stability. In this research, acoustic emission (AE) has been used to monitor events occurring within Si/Li foil half cells during both constant current-constant voltage (CCCV) and cyclic voltammetry (CV) tests. CCCV between 50mV-1.3V showed the greatest amount of AE activity on the first Li intercalation with each subsequent cycle delivering progressively fewer emissions. SEM showed deep cracks and particle fractures. When CCCV was limited between 170mV-1.3V significantly fewer emissions were recorded and no notable particle damage was observed. CV testing at 0.05mV/s between gave AE activity only on Li intercalation at low potentials. SEM of these samples shows extensive surface cracking and peeling on the particle surface.

Neutron Diffraction Measurements of Residual Stresses in Bent Stainless Steel Pipes: *Mihyun Kang*[1]; Wanchuck Woo[1]; Vyacheslav Em[1]; Hyoung Seop Kim[1]; Sun Ig Hong[1]; Baek-Seok Seong[1]; Kye Hong Lee[1]; [1]KAERI (Korea Atomic Energy Research Institute)

Owing to the extraordinary anti-corrosion and high strength properties, stainless steels have been widely used for the structural materials in nuclear power plants. In many designs and applications, bending of the pipes is inevitable and the residual stresses can be detrimental to the integrity of the end products. In this study, we investigated the distributions of the residual stresses from bent 304 stainless steel pipes using neutron diffraction. A total of four seamless pipes, as-received state (without bending) and bent with the three different bending curvatures (R = 250,500 and 750 mm), have been prepared. Each pipe specimen was installed in the residual stress diffractometer at HANARO (High-flux Advanced Neutron Application Reactor), KAERI (Korea atomic energy research institute) and the residual stresses were measured at several different locations of pipes. The neutron diffraction results will be also compared to the computational simulation results calculated using the finite element method.

Numerical Simulation of Alumina Sintering: *Mohammed Kadhim*[1]; [1]University of Technology

Sintering process has been analysed mathematically by prediction unsteady-state mathematical model in order to give more description and understanding for the mechanism of this process. This includes mass transport phenomena which may occur via diffusion.The spatial and temporal temperature profile with the solid medium has been determined by solving the unsteady state Fourier heat energy transport equation using the explicit finite difference numerical method, which would minimize the solution errors. This has been lead to more realistic determination of temperature distribution within the work-piece. Alumina has been selected as a target to represent nonmetallic material of diverse physical and thermal properties. The average grain size for alumina powder is 0.5 µm with initial compact density 2160 kg/m3. These values gave a reliable approach to calculate the porosity and relative strength. The porosity is a function of density and relative strength, so the porosity decreases with increase in the density.

On the Role of Pieirls Stress in the Shock Response of Cubic Metals: *Neil Bourne*[1]; [1]AWE

The response of four cubic metals to shock loading is reviewed in order to understand the effects of microstructure on continuum response. Experiments are described that link defect generation and storage mechanisms at the mesoscale to observations in the bulk. The behaviours described are linked through description of time-dependent plasticity mechanisms to the final states achieved. Recovered targets displayed dislocation microstructures illustrating processes active during the shock loading process. Lower symmetry metals possess high Peierls stress and thus have higher resistances to defect motion in the lattice under shock loading conditions. These behaviours illustrate the role of defect generation, transport, storage and interaction in determining the response of materials to shock prestraining.

Oxidation and Ignition Resistances of AM60B-Based Eco-Mg Alloys: *In-Kyum Kim*[1]; Jung-Ho Seo[1]; Shae K. Kim[1]; [1]Korea Institute of Industrial Technology

This paper focuses on the possibility to improve oxidation and ignition resistances of CaO added Eco-Mg alloys based on AM60B with good elongation, ductility and high-pressure die-castability. It has been already confirmed by the previous studies that the oxidation and ignition resistances of CaO added AZ31 and AZ91 are improved by the small addition of 0.3wt.% CaO. The purpose is to optimize CaO contents not only for improving the oxidation and ignition resistances but also for maintaining the alloy's process-abilities and mechanical properties, esp. elongation, on the basis of non-SF6 gas processing. Varying amounts of CaO (0.1, 0.3 and 0.5wt.%) were added into AM60B and the prepared alloys were gravity-cast into a metallic mold. The oxidation resistance was examined through TGA. The ignition resistance was examined by DTA under dry air atmosphere. The AES depth profile was performed to evaluate the ignition resistance in terms of surface oxide stability.

Oxidation Behavior of ZrB2-ZrO2 Composites Prepared by Spark Plasma Sintering: *Lian Zhang*[1]; Junguo Li[1]; Jianrong Song[1]; Huiping Yuan[1]; Chuanbin Wang[1]; Qiang Shen[1]; [1]Wuhan University of Technology

ZrB2-ZrO2 composites were prepared by spark plasma sintering at 1900° from ZrB2 powders which were coated by and mixed with ZrO2-3mol%Y2O3, repectively. The composites were then oxidized at 1200° for 240 min and the phase, microstructure and weight change of the samples, before and after oxidation, were investigated. For the samples prepared from the mixed ZrB2-ZrO2 powders, macro-cracks appeared on the sample surface and oxygen diffused rapidly through these cracks, leading to the fast oxidation of ZrB2 grains. However, the oxidation rate of the composites prepared from coated ZrB2 powders was decreased remarkablely and they showed good resistance to oxidation. The main phase of the coated ZrB2-ZrO2 composites was ZrB2 with a small amount of t- and m-ZrO2, even after oxidation for 4 hours. No crack was dicerned on the sample surface, and as a result oxygen diffused hardly through the ZrB2 grain boundary.

Phase Decomposition during Aging in an Al-22wt.%Zn Alloy: Lizbeth Melo-Maximo[1]; Dulce Melo-Maximo[1]; Susana Lezama-Alvarez[1]; Erika Avila-Davila[2]; *Victor Lopez-Hirata*[1]; Orlando Soriano-Vargas[1]; Jorge Gonzalez-Velazquez[1]; [1]Instituto Politecnico Nacional (ESIQIE); [2]Instituto Tecnologico de Pachuca

This work shows a study of morphology and growth kinetics of the phase decomposition as well as its effect on the hardening behavior during the aging at 373 and 393 K in an Al-22wt.%Zn alloy. The aging process was analyzed using a solution of the nonlinear Cahn-Hilliard equation by the explicit finite difference method. Besides, the aging process was studied by XRD, TEM and Vickers hardness of the aged Al-22wt.%Zn alloy. The numerical simulation results showed the supersaturated solid solution decomposed spinodally into a mixture of Al- and Zn-rich phases after aging. Simulation and TEM results showed that the morphology of the decomposed phases was irregular and interconnected and it changed to rounded particles as aging progressed. The increase in hardness is related directly to the formation of the decomposed phases during aging of this alloy.

Plasma-Polymerization of Hexamethylcyclotrisiloxane Using Atmospheric Pressure Dielectric Barrier Discharge: *Gi Taek Kim*[1]; Yoon Kee Kim[1]; [1]Hanbat National University

In this work, we have tried to deposit organosilicon layers from hexamethylcyclotrisiloxane (HMCTSO) using helium DBD generated by 30 kHz AC at atmospheric pressure. The compositions of organosilicon layers have been controlled from SiOC to SiO_2 by changing flow rates of the carrier gas and oxygen. The O_2/ HMCTSO-He carrier gas flow ratios ranged from 1:2 to 1:20 and the coatings have been grown with deposition rates in the range from 200nm/min to 800nm/min. The coatings exhibit Si-O bonding and Si-CH_3 bonding. The Si-O bonding was increased with the O_2/ HMCTSO-He carrier gas flow ratio and finally, silicon to oxygen ratios are approximately 1:2 with some incorporated carbon. We will discuss the effects of the composition of source gases on the surface morphologies and bonding structures of the films.

Prediction of Rapid Solidification Nanosize Structure for Aluminium Alloys: *S. Valdez*[1]; [1]UNAM-ICF

The purpose is to develop a principle based on kinetic and thermodynamic solidification theory in order to predict the rapid solidification nanosize structures to be applied at aluminium alloys. Thermodynamic considerations are based in the thickness of the solidified layer, which must be known in order to calculate the heat flux per unit time to the chill substrate. Considering that the cooling condition in melt spinning is controlled by the melt/substrate interface (Newtonian cooling). In addition, the equilibrium phase diagram has been used as well as assumptions based in the Scheil Solidification Model. For rapid solidification theory, is considered that the Local equilibrium exists at the solid/liquid interface, No diffusion in the solid phases, Uniform liquid composition and No density difference between solid and liquid.

Preparation and Characterization of Nanocrystalline Silver Particles: *Burcak Ebin*[1]; Elif Yazici[1]; Sebahattin Gurmen[1]; Burak Ozkal[1]; [1]Istanbul Technical University

Silver particles are widely used as antibacterial/microbial agent in medical, cosmetic, textile and marine sectors. They are also an important substance of conductive inks, paste, sensors and various electronic devices due to their physicochemical properties that can be controlled by size in nanoscale. In this research, nanocrystalline Ag particles were prepared by ultrasonic spray pyrolysis (USP) method using silver nitrate aqueous solution. The dependence of morphology, particles and crystalline sizes to the carrier gas (H2, N2 and air) were investigated under 1.0 l/min gas flow rate, 0.1M precursor concentration, 600°C reaction temperature and 1.3 MHz ultrasonic frequency conditions. Scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS) and X-ray diffraction (XRD) were used to investigate size, morphology and crystal structure of particles. It was observed that nanocrystalline spherical Ag particles obtained in all conditions with crystalline sizes are nearly 39 nm which are calculated by Schrrer equation.

Preparation of Iridium Fine Particle by the Effect of Grinding Additive, NaCl: *Young Jin Kim*[1]; Youngsan Ham[1]; Jaeryeong Lee[1]; [1]Kangwon National University

Grinding of the mixture, Ir(Iridium) and NaCl(Sodium chloride), was carried out for the preparation of Ir fine powders. For the Grinding for only Ir, the structure of Ir was defected and also the abrasion from the pot and balls was input the ground mixture due to the intensive grinding. On the case of grinding with NaCl, the crystalline of Ir was kept and the abrasion was suppresed considerably. The fine Ir with a size of 1~3 µm can be prepared by the washing process for the ground with mixture.

Pressurless Sintering of Al2O3-SiC Nano Composites and Effect of Additives on Sintering Temperature: *H.R. Rezaie*[1]; [1]Iran University of Science and Technology

Al2O3-SiC nano composite ceramics were prepared by pressureless sintering with or without the addition of Y2O3, MgO and TiO2 as sintering aids. The effects of these compositional variables on sintering rate and final density were investigated. The addition of 5 vol.% SiC to Al2O3 hindered densification. In contrast, the addition of Y2O3, MgO and TiO2 to Al2O3–5% SiC nanocomposites improved densification. Al2O3 and SiC nano powders that were produced separately by sol gel method in previous work were used in this part as starting materials. Green bodies were obtained by uniaxual pressing of 200 MPa.Pressureless sintering was carried out in a nitrogen atmosphere at 1600°C and 1630°C.Maximum density (97%) was achieved at 1630°C. Vickers hardness 18GPa after sintering at 1630°C. Scanning electron microscopy revealed that the SiC particles were located predominantly to the interior of the matrix grains and well distributed throughout the compositemicrostructures.

Process Modeling for Synthesis of Metal Matrix Nanocomposites: *Payodhar Padhi*[1]; Biranchi Dash[2]; [1]Hi-Teh Medical College & Hospital; [2]Konark Institute of Science & Technology

The present study models the processing of metal matrix nanocomposites in a solidification rout, where the dispersion of nano ceramic particles in the liquid aluminum melt during the cavitation process. High-intensity ultrasound is used for mixing, dispersing and deagglomeration of the fine particles in the liquids. The model simulates the effect of pressure shock wave generated as a result of periodic collapsing of bubbles at a location on particle distribution within adjacent agglomerate of nano-particles. This model will demonstrate the phenomenon of deagglomeration and dispersion. In the model a combination of Eulerian multiphase and turbulence model will be used which solves a set of momentum and continuity equations for each phase. Coupling is achieved through the pressure and interphase exchange coefficients. The distribution of nano ceramic particles in the melt liquid during the process of metal matrix nanocomposites has been studied.

Producing of Composite Layer of TiO2/Al5083 via Friction Stir Processing: *Reza Behnagh*[1]; Mohamm Kazem Besharati[2]; [1]Tehran University; [2]Department of Mechanical Engineering, Tehran University

Friction stir processing is a solid state process to modify microstructure and mechanical properties of sheet metals and as-cast materials. In this process stirring action of the tool causes the material to intense plastic deformation that yields a dynamical recrystallization. In this study the effect of FSP and process parameters on hardness, and microstructure of Al5083 has been investigated. Also by using of FSP, composite layer of TiO2/Al5083 has been produced. Results show that, FSP leads to finer and homogenized grain structure, as well as increased hardness, strength, toughness, and elongation of material. The composites produced by FSP have uniformly distribution of TiO2 particles between the grains of base metal.

Production of Boron Fiber in a CVD Reactor: *Selim Ertürk*[1]; Ismail Duman[1]; [1]Istanbul Technical University

Boron fibers are special yarns, having a diameter of 100-130 microns that are produced by chemical vapor deposition (CVD) process on tungsten filament (φ 10-15 microns) as the core material. A glass reactor used as CVD medium (30 cm length and 10 mm ID / 12 mm OD) was designed to investigate the optimum production conditions of boron fiber production by the reaction of borontrichloride and hydrogen gases. Reaction temperature is controlled by heating the tungsten substrate (wire) via mercury-indium amalgam. An FT-IR spectrophotometer is connected to the exhaust of the reactors to perform online chemical analysis of the effluent gas mixture. Experiments were carried out at atmospheric pressure and at a reaction temperature range of 800-1250 °C with different inlet reactant concentrations. According to production conditions, mechanical and chemical properties of the boron fibers were investigated.

Production of Porous, Intermetallic Titanium Aluminide Reinforced Titanium Matrix Composites by Powder Metallurgy Method: Aydin Bicer[1]; *Eyup Kayali*[1]; Huseyin Cimenoglu[1]; [1]Istanbul Technical University

In this study, intermetallic titanium aluminide reinforced titanium matrix composites were produced by conventional powder metallurgy method (i.e cold pressing and sintering). Composites produced directly from titanium (70wt%) and aluminum(30wt%) powder mixtures provided porosity (37%) consist of micropores formed by intermetallic transformation in the microstructure, while involving high compressive strength values (69MPa). In the present study porosities were increased by putting volatile polymer powders into mixture as additive and presintering at volatilizing tempretaure. When volatilizing (presintering) process performed, pores with same particle size took place of polymer powders in addition to smaller pores formed by intermetallic transformation during liquid phase sintering process at 700ºC. Due to having two types of pores which have different particle size also provided an advantage of allowing interconnection. The structure was not only highly porous but also had remarkable compressive strength (23MPa) to maintain that sufficient porosity (63%).

Production of Titanium Carbide Reinforced Titanium Matrix Composites via Powder Metallurgy Method: *Burak Karaduman*[1]; Onur Meydanoglu[1]; Huseyin Cimenoglu[1]; Eyup Kayali[1]; [1]Istanbul Technical University

In this study titanium carbide reinforced titanium matrix composites were produced by conventional powder metallurgy method. Titanium powders were mixed with graphite powders at different compositions. Composites produced directly from titanium and graphite powder mixtures provided high amount of porosity in the microstructure, while involving high hardness values. In the present study porosities were eleminated by a two step process. As the first step bulk titanium carbide was produced from titanium and graphite powder mixture. In the second step porosity free titanium matrix composites were produced by utilizing the mixture of titanium carbide and titanium powders. In order to determine the effect of hot pressing on microstructure titanium and graphite mixtures were hot pressed at 1300C under vacuum conditions. Microstructural examinations, hardness measurements and wear tests were conducted on composites. Although relative densities of composites decreased, higher hardness values and wear resistances were obtained as titanium carbide content increased.

Properties and Performance of Composites Based on Superrefractories Cements: *Ilyoukha Nickolai*[1]; Timofeeva Valentina[1]; [1]Academic Ceramic Center

Superrefractories cements (1800-2700°C) is a new refractory insulating material and objective of this work is to enlarge our knowledge about this new product and to search solutions for problems the industry is facing. Based on this target, we realized several test to find answers to important questions about the application of this product in severe industrial conditions and to analyze how this material performs in high temperatures. High temperature composites and coatings based on superrefractories cements are meant to protect units from influence of temperature more than 2000°C and used for manufacturing monolithic lining, crucibles used in the melting of pure metals, including alloys on rare-earth elements, for closing one of ceramic modules of fire wall, in refractory lining of quartzglasstanks, petrochemistry reactors, H2, furnaces, carbon reactors in burial of radiation wastes by extreme environments.Key words: composites materials, properties, performances, cements reactors, temperature.

Properties and Rapid Consolidation of Nanostructured Ti from Mechanically Activated Ti and Tih2 By High Frequency Induction Heated Sintering: *In-Jin Shon*[1]; Na-Ri Kim[1]; In-Yong Ko[1]; Je-Shin Park[2]; Wonbaek Kim[2]; [1]Chonbuk University; [2]Korea Institute of Geoscience and Mineral Resources

Titanium has a good deformability, high hardness, high biocompatibility, excellent corrosion resistance and low density. Due to these attractive properties, it has been used in many industrial applications. Dense nanostuctured Ti was sintered from mechanically activated Ti and TiH2 powders by the high frequency induction heated sintering under pressure of 80Mpa, respectively. TiH2 powder was decomposed to Ti during the sintering. The hardness of Ti increased and the average grain size of Ti decreased with increasing milling time. The average grain sizes of Ti sintered from Ti powder and TiH2 powder milled for 5hrs were about 17nm, 28nm, respectively. The hardness and fracture toughness of Ti sintered from Ti powder and TiH2 powder milled for 5hrs were 504kg/mm2, 567kg/mm2 and 7MPa•m1/2, 7MPa•m1/2, respectively.

Properties and Rapid Consolidation of Nanostructured Tasi2 from Mechanically Synthesized Powder by High Frequency Induction Heating: *In-Jin Shon*[1]; Seung-Myoung Chae[1]; In-Yong Ko[1]; Jin-Kook Yoon[2]; Kee-Do Woo[1]; [1]Chonbuk University; [2]Korea Institute of Science and Technology

TaSi2 has an attractive combination of properties, including high melting temperature, high modulus, high oxidation resistance in air, and a relatively low density. To improve on its mechanical properties, the approach commonly utilized has been the addition of a second phase to form composite and to make nanostructured materials. Nanopowder of TaSi2 was synthesized from Ta and 2Si powder during the high energy ball milling for 20hrs. Dense nanostructured TaSi2 was consolidated by high frequency induction heating within 2 minutes from mechanically synthesized powders of TaSi2. Highly dense TaSi2 with relative density of up to 98% was consolidated under simultaneous application of a 80 MPa pressure and the induced current. The average grain sizes of TaSi2 were about 33 nm. The average hardness and fracture toughness values obtained were 1330 kg/mm2 and 3.3 MPa•m1/2, respectively.

Qualitative Analysis of Temperature Evolution in Railway Brake Disc: *Jeongguk Kim*[1]; Sung-Tae Kwon[1]; Sung Cheol Yoon[1]; Byung Choon Goo[1]; [1]Korea Railroad Research Institute

In order to analyze the degradation mechanism of brake disc, the qualitative analysis of surface temperature changes on railway brake disc was conducted using a high-speed infrared camera. The infrared camera employed for this investigation has max speed of 380 Hz. The braking tests with the railway brake disc were performed with a full scale dynamometer, and the high-speed infrared camera was used to monitor surface temperature changes on the brake disc during the braking test. Through the analysis of thermographic monitoring images, the temperature evolution with different braking speeds was qualitatively evaluated, and the results showed the initial thermal bands on brake disc was formed at relatively low braking speed, and the localized hot spots were observed at the braking speed of 180 km/h. In this paper, the qualitative investigation results on the temperature evolution of railway brake disc was summarized and presented.

Quality and Productivity Improvements for Wire and Cable Industry: *Kiran Manchiraju*[1]; [1]Southwire Company

Abstract: Significant quality and productivity improvements can be made to wire and cable products if porosity is detected and eliminated during the casting of copper rod. A system that detects porosity, during the continuous casting (CC) of copper bar has been developed. This system uses an infrared red camera that measures surface temperature as the copper bar exits the casting wheel and after cooler. A statistical algorithm that uses the temperature profile from the IR camera has been developed that reveals the existence or absence of porosity within the CC bar. The temperature profile is curve fitted to an nth degree polynomial and is then evaluated by analyzing the residuals at peak temperatures. Using the procedures advanced above, bar porosity less than 1/8th of an inch in diameter have been detected at the Southwire Carrollton facility.

Quality Control of the Refining Process at Electron Beam Melting and Development and Implementation of Engineering Support System for Process Modeling and Control: *Elena Koleva*[1]; Georgi Mladenov[1]; Idilia Batchkova[2]; Kamen Velev[2]; Vania Vassileva[1]; Katia Vutova[1]; [1]Institute of Electronics - Bulgarian Academy of Sciences; [2]University of Chemical Technology and Metallurgy

The behavior of various impurities in the crystallized ingots and the evaporated base metal losses at Electron Beam Melting and Refining (EBMR) of Ti, Cu and some refractory metals are analyzed. Experimental kinetic dependencies of impurity concentrations are estimated. Simulation of the thermal processes is used for some parameter estimation at EBMR. Statistical methods are applied for the quality improvement of the obtained ingots. Optimization of the EBMR regime conditions is performed aiming improving the quality of the obtained ingots (including the variations and the repeatability of the results) and minimization of base metal evaporation losses. The developed Engineering Support System (ESS) for EBMR plant is briefly described. The system is intended to integrate and organize the knowledge for the EBMR, to serve modeling, control system design and simulation of EBMR and complementary production processes (either continuous or discrete) connected to the industrial needs for efficiency, adaptability, flexibility and reconfigurability.

Quality of Slab Ingots and Heavy Plates Produced by a 40t ESR Furnace: *Xin Geng*[1]; Zhouhua Jiang[1]; [1]Northeastern University

The research on the refining and solidification in a large bifilar ESR furnace for production of slabs up to 40t are performed. The gross segregation experiments were carried out to check the uniformity of components of heavy plates in different position. The slab ingots were rolled to heavy plates, and then the impact toughness and tensile properties of heavy plates produced by an ESR furnace for slab products with different position were compared with that of heavy plates produced by a conventional process. The suitable refining and solidification process was obtained during the ESR for slab ingots. Adjusting taper of the mold and using CaF2-CaO-Al2O3-SiO2-MgO slag are necessary to improve surface quality of the ESR slab. The gross segregation results show that the heavy plates produced by ESR furnace exhibits excellent uniformity. And the mechanical properties of the heavy plates are superior to that of conventional materials.

Rapid Consolidation of Nanocrystalline 2Fe-Al2O3 Composite from Mechanically Alloyed Powders by Pulsed Current Activated Sintering: *In-Jin Shon*[1]; Dong-Mok Lee[1]; Na-Ra Park[1]; Na-Ri Kim[1]; Je-Shin Park[2]; Wonbaek Kim[2]; [1]Chonbuk University; [2]Korea Institute of Geoscience and Mineral Resources

Metal matrix composites combine metallic properties (ductility and toughness) with ceramic characteristics (high strength and modulus), leading to greater strength in shear and compression and to higher service temperature capabilities. The attractive physical and mechanical properties that can be obtained with metal matrix composites, such as high specific modulus, strength-to weigh ratio, fatigue strength, and temperature stability and wear resistance, have been documented extensively. Nano-powders of Fe and Al2O3 were synthesized from Fe2O3 and 2Al powders by high energy ball milling. Nanocrystalline 2Fe-Al2O3 composite was consolidated by pulsed current activated sintering(PCAS) method within 2 minutes from mechanically alloyed powders of Al2O3 and 2Fe. The average grain sizes of Fe and Al2O3 in the composite were 150 nm and 86 nm, respectively. The average hardness and fracture toughness values obtained were 1202 kg/mm2 and 12 MPa•m1/2, respectively.

Rapid Solidification of FeAlCr-B2 Intermetallic Compounds - Microstructure and Mechanical Behavior: *Roberto Rodriguez-Diaz*[1]; Julio Juarez-Islas[2]; Jesus Arenas-Alatorre[3]; [1]Facultad de Quimico-Metalurgica UNAM; [2]IIM_UNAM; [3]Instituto de Fisica - UNAM

This work presents microstructural characterization of a melt-spun intermetallic compound Fe40Al5Cr (% at.), produced by rapid solidification employing the melt spinning technique at different wheel speeds. Microstructure and structure features in ribbons were characterized by optical and scanning electron microscopy (SEM), x-ray diffraction analyses (XRD) Transmission electron microscopy (TEM) and EDS technique was employed to perform point and scan line chemical analyses. Micro hardness Vickers measurements as well as tensile tests at room temperature were applied to ribbons. The grain size of rapidly solidified Fe40Al5Cr ribbons suffered a drastic reduction as compared with those alloys in as-cast state. Grain size of as-spun ribbons decreased as the wheel speed or cooling rate increased. Hardness measurements revealed a softening in rapidly solidified FeAlCr ribbons as compared with FeAl alloys and tensile test exhibited a (transgranular + intergranular) mode of fracture, reaching up to 3 % of elongation in FeAlCr alloys.

Recovery of Metallic Values from Spent Li Ion Secondary Batteries: *Serdar Aktas*[1]; Derek Fray[2]; Jo Fenstad[2]; Odna Burheim[2]; Ercan Acma[1]; [1]Istanbul Technical University; [2]University of Cambridge

Recovery of metallic values from spent Li ion batteries by a precipitation technique using ethanol was investigated. Cobalt was recovered in two steps. During the first step, 92% of the cobalt was recovered as CoSO4 by the use of ethanol at a volume ratio of 3 : 1. In the second step, the remaining cobalt was precipitated as cobalt hydroxide by increasing the pH value with the addition of lithium hydroxide. Lithium, which remained in the solution, was then recovered as lithium sulphate with up to 90% recovery efficiency by the addition of ethanol at a 3 : 1 volume ratio. It was found that the ethyl alcohol was capable of removing water ligands from cations, resulting in the precipitation of metals as metal sulphate monohydrate. It was shown that metals could be precipitated separately by the ethanol/sulphate precipitation technique depending on their concentrations present in the solution.

Removal of Phosphorus from High-Phosphorus Iron Ores by Selective HCl Leaching Method: *Wentang Xia*[1]; Xingyu Chen[2]; Zhengde Ren[1]; Ailiang Chen[2]; Yifeng Gao[1]; Tongguo Wang[1]; [1]Chongqing University of Science and Technology; [2]Central South University

The selective HCl leaching method was used to remove phosphorus from high-phosphorus iron ores.The hydroxyapatite in high-phosphorus iron ores was converted into soluble phosphate during the process of HCl leaching. The effects of reaction time, particle size, hydrochloric acid concentration, reaction temperature, liquid-solid ratio and stirring speed on the dephosphorization ratio were studied.The results showed the dephosphorization ratio can exceed 98% on the conditions of reaction time 30-45 min, particle size 0.074-0.104 mm, hydrochloric acid concentration 2.5mol/L, reaction temperature 25°, liquid-solid ratio 5/1 and stirring speed 150-250r/m. After dephosphorization reaction, the content of phosphorus in iron ore accorded completely with requirement of steel production.

Rhodium Recovery from Spent Rhodium Plating Solutions: *Bihter Zeytuncu*[1]; Serdar Aktas[1]; Hakan Morcali[1]; Onuralp Yucel[1]; [1]Istanbul Technical University

In this study, recovery of rhodium from spent rhodium plating solutions via cementation was investigated. Rhodium, a member of the platinum group metals, is used for decorative purposes, and in most cases is preferred to silver since it does not tarnish under moderate conditions unlike silver. For recovery experiments, fine metallic aluminum, zinc and iron powders were employed, and their recovery efficiencies were compared to each other. It was found that increasing temperature plays an important role in the recovery of rhodium as well as in the reaction time. When the same amount of cementator was employed zinc was found to be more successful in attaining higher recovery efficiencies than aluminum and iron, which can be attributed to the fact that aluminum and iron are more prone to oxidation than zinc powder. It was shown that these three cementators are capable of precipitating rhodium from spent plating solutions quite effectively.

Rotary Ultrasonic Drilling of Al2O3 Ceramic Material: *Naga Prasada Rao Boyalapalli*[1]; Laxminarayana Pappula[2]; M. Ramulu[3]; [1]Department of Mechanical Engineering, University College of Engineering, Osmania University; [2]University College of Technology, Osmania University; [3]Department of Mechanical Engineering, University of Washington

Ultrasonic Machining (USM) can effectively machine hard and brittle materials such as ceramics but it has the disadvantage of a low material removal rate. It was found in this study that the material removal rate can be substantially increased by applying a rotating motion to the work piece during machining. The increase in material removal rate can be four times greater than the rate achieved without rotation (conventional USM). Polynomial models of the resulting material removal rate and tool wear rate were made. The relationship between parameters and response was examined. Optimum parameters for maximum material removal rate and for minimum tool wear rate were also found. The Taguchi method was used in combination with regression analysis to find robust process parameters that would satisfy the objective of reducing the influence of noise factors by controlling the controllable factors thereby maximizing MRR and minimizing TWR.

Scrap Modified Alloy Design of Wrought Aluminum Alloy: *Myoung-Gyun Kim*[1]; [1]Research Institute of Industrial Science and Technology(RIST)

Saving of resource and energy is very important for establishing the sustainable environment. The developments of materials processing and recycling for light metals, especially, aluminum alloys, are very useful for the materials and energy saving in various industries. Because aluminum scrap, in particular, contains iron-containing parts, such as bolt, nut, etc., in remelting or recycling aluminum scrap, it is essential to develop the technique removing iron in aluminum melts. It is well known that the intermetallic-AlFeSi phase that forms needle shape during the solidification of aluminum alloys is detrimental to extrusion properties owing to increasing of extrusion pressure. In this study, we are going to modified alloy design wrought (5000, 6000, 7000 base) aluminum alloy using aluminum scrap. To develop scrap modified alloy design of wrought aluminum alloy, both computer simulation and experimental results are discussed.

SEM Analysis of Worn Carbon Cathodes in Industrial Aluminium Electrolysis Cells: *Øyvind Østrem*[1]; Christian Rosenkilde[2]; [1]Norwegian University of Science and Technology; [2]Norsk Hydro ASA

Wear of the carbon cathode is the main limiting factor for the life span of aluminium electrolysis cells. The wear profile is often very uneven with areas in the middle of the cell showing little wear while at the sides and edges the cathode can be worn down to the current collector bars. A more even wear could give a prolongation of the life span by several years, which obviously can be a significant economic advantage. This work focuses on microscopy analysis of surface samples of cathodes in industrial aluminium electrolysis cells. The objective is to thoroughly study the metal cathode interphase to determine if there are visible differences in the surface from areas with little wear compared to the surface from areas with more wear. Any differences, together with the surface study itself, may give indications to what wear mechanisms the carbon cathode is subjected to during aluminium electrolysis.

Silver Recovery from Silver-Rich Photographic Processing Solutions by Copper: *Bihter Zeytuncu*[1]; Hakan Morcali[1]; Serdar Aktas[1]; Onuralp Yucel[1]; [1]Istanbul Technical University

The present study investigates silver recovery from silver-rich photographic processing solutions by copper. The effects of various reaction parameters on silver recovery efficiency were studied in detail. Parameter optimization was also carried out. The possibility of recovering silver with more than 99% efficiency was demonstrated under both air and argon atmospheres. In the latter case, more than 99% recovery efficiency was achieved at an agitation rate of 875 rpm for 8 minutes. When cementation was carried out under air, the silver recovery efficiency decreased with increasing time, and agitation rate. This decrease can be attributed to the redissolution of cemented silver back into the solution. In addition, the solution pH was demonstrated to influence the efficiency of silver recovery by copper.

Silver Recovery from Waste Radiographic Films Using Different Methods: *Hakan Morcali*[1]; Serdar Aktas[1]; Onuralp Yucel[1]; [1]Istanbul Technical University

A chemical processing scheme was adopted to recover silver from waste radiographic films. The films were subjected to 1 M nitric acid solution for 3.5 hours at 80°C. The silver nitrate solution was then treated by two different methods. The first involved cementation with iron and zinc powders. These cementators were compared to each other with respect to purity of the final product and the recovery efficiency. The second method was sodium hydroxide precipitation. The treatment with Fe and Zn powders resulted in the formation of metallic silver in just one step; silver oxide obtained via NaOH precipitation was subsequently treated by two different methods: a treatment with a mixture of glucose and NaOH to yield metallic silver, and a heat treatment, in which Ag2O was converted to silver at 500°C. With the exception of the powder produced by glucose reduction, all the other powders would easily find industrial application.

Simulation of Dislocation Interaction with Precipitates: *Peihua Jing*[1]; Hyon-Jee Lee[2]; Jae-Hyeok Shim[3]; Ian Robertson[4]; Brian Wirth[2]; [1]Structural Integrity Associates; [2]Department of Nuclear Engineering, The University of California, Berkeley; [3]Korea Institute of Science and Technology; [4]Department of Material Science and Engineering, The University of California, Berkeley

Molecular Dynamics (MD) simulations of an edge dislocation interacting with several obstacles have been analyzed in terms of the partial dislocation reactions using Thompson tetrahedron notation. These include an oversize {100} platelet and a self-interstitial [001] loop, and the results provide a basis to understand the interaction between an edge dislocation and non-coherent precipitates. In all cases, the MD simulations reveal more complicated interactions between the dislocation and non-coherent precipitates than theoretically anticipated. For an oversized Au precipitate, the interaction involves a combination of Orowan looping plus absorption and subsequent dragging of a dislocation loop segment. For an undersized in-coherent Rh precipitates, numerous Shockley partial dislocation loops were nucleated at the precipitate – matrix interface as the dislocation approached, thereby significantly increasing the obstacle strength.

Simultaneous Synthesis and Consolidation of Nanostructured Ti-ZrO2 from Mechanically Activated Powders by High Frequency Induction Heated Combustion: *In-Jin Shon*[1]; Seung-Myoung Chae[1]; Je-Shin Park[2]; Wonbaek Kim[2]; Kee-Seok Nam[3]; [1]Chonbuk University; [2]Korea Institute of Geoscience and Mineral Resources; [3]Korea Institute of Materials Science

Interest in cermet of Ti-ZrO2 has increased significantly in recent years because of their potential application as aeronautical and automotive materials. This combination of metal and ceramic has good properties, such as adequate creep resistance at high temperature, low density, excellent oxidation and corrosion resistance, good wear resistance and high hardnessDense nanostructured Ti-ZrO2 composite was synthesized by high frequency induction heated combustion synthesis(HFIHCS) method within 2 minutes in one step from mechanically activated powders of TiO2 and Zr. Highly dense Ti-ZrO2 with relative density of up to 99% was simultaneously synthesized and consolidated under application of a 80 MPa pressure and the induced current. The average grain sizes of Ti and ZrO2 in the composite were 26 nm and 21 nm, respectively. The hardness and fracture toughness of the composite were 1041 kg/mm2 and 10 MPa.m1/2, respectively.

Sintering Behaviors of ZrC Nanoparticle Dispersed Tungsten Based Composites: *MinKyung Kim*[1]; HyunJu Choi[1]; DongHyun Bae[1]; [1]Yonsei University

ZrC/W composites have been received a growing attention for aerospace applications requiring ablation resistance, creep resistance and toughness at extremely high temperature (= 2000°C); ZrC particles could be turned into ZrO2 layers at high temperature and the oxide layer could effectively hinder the oxidation of tungsten. In this study, ZrC/W composites have been fabricated using mechanical milling and sintering. Planetary ball milling has been used to disperse ZrC particles in the tungsten powders. As milling was processed, the brittle ZrC particles could be fragmented to be hundreds nanometer-sized and homogenously distributed in the tungsten powders. By controlling the sizes of tungsten powders in the range from 1μm to 20 μm, the distribution of ZrC particles in the composites was observed. The effects of the particle morphology on the sintering process will be also discussed.

Sintering Densification and Microstructural Characterization of Mechanical Alloyed Fe-Mn-Si Based Powder Metal System: *Ahmet Söyler*[1]; Burak Özkal[1]; Leandru Bujoreanu[2]; [1]ITU; [2]"Gh. Asachi" Technical University from IASI

In this study sintering behaviour of Fe-Mn-Si based powder metal system were investigated using vertical dilatometer. Grain size refinement of key target composition alloys performed via mechanical alloying by taking advantage of high energy milling equipment. Both powder state and sintered state phases were characterized via XRD studies and effect of mechanical alloying time against sintering densification of Fe-Mn-Si based powder metal system were investigated for the different sintering regimes and atmospheres.

Sintering Kinetics of SPS Tungsten and Tungsten-Ceria Cermets: Jeffrey Perkins[1]; Kyle Knori[1]; *Darryl Butt*[1]; [1]Boise State University

The spark plasma sintering (SPS) method was used to consolidate tungsten powders and tungsten-ceria powders. Sintering temperatures, dwell times, pressures, and ceria content were varied to study the densification kinetics and grain growth kinetics of these parts. The sintering kinetics was evaluated based on the densities, porosities, grain sizes, and sintering displacement rates of the parts. The growth of tungsten grains was inhibited by small additions of ceria, and larger additions of ceria had a limited effect on tungsten grain growth. No diffusion was observed between the tungsten and the ceria. At higher temperatures, ceria was reduced during sintering, causing pores to be formed in the resulting microstructure. Based on the kinetics data, potential sintering mechanisms of tungsten and tungsten-ceria in SPS are proposed.

Small Punch Creep of Service-Exposed SUS 316 HTB Superheater Tubes of Fossil Boilers: *Maribel Saucedo-Muñoz*[1]; Shin-Ichi Komazaki[2]; Toshiyuki Hashida[3]; Toru Takahashi[3]; Victor Lopez-Hirata[1]; Tetsuo Shoji[3]; [1]Instituto Politecnico Nacional (ESIQIE); [2]Muroran Institute of Technology; [3]Tohoku University

The creep properties for a SUS 316 HTB austenitic stainless steel were evaluated by using the small-punch creep test at 650°C and loads of 234, 286, 338, 408 and 478 N, and at 700°C and loads of 199 and 234 N. The creep curves, determined by means of the small punch creep test, were similar to those obtained from a conventional uniaxial creep test. That is, they exhibited clearly the three creep stages. The width of secondary creep stage and rupture time tr decreased with the increase in testing load level. This difference in creep resistance was explained based on the difference in the creep deformation and/or fracture mechanism. It was also found that the ratio between the load of small-punch creep test and the stress of uniaxial creep test was about one for having the same value of creep rupture life.

Some Recent Research Work on the Hot Processing of Engineering γ-TiAl Alloys: *Yuyong Chen*[1]; Yanfei Chen[1]; Shulong Xiao[1]; Fantao Kong[1]; Jing Tian[1]; [1]Harbin Institute of Technology

TiAl alloys have attracted a major effort in lightweight structural components for aerospace and automotive applications because of their favorable properties of high specific strength and temperature capability over the past 20 years. The paper outlines some recent research work on the hot processing of engineering TiAl alloys through ingot metallurgy technology including investment casting and sheet rolling at our laboratory. Ingots and castings of TiAl alloys are prepared by ISM in a water cooling copper crucible. TiAl blades and rudder frame work were successfully produced by investment casting using a newly developed ceramic mold. And Ti-43Al-9V-0.3Y sheets were obtained with hot rolling of canned forged TiAl alloys in α+γ zone. Some concerns in producing the TiAl castings and sheets will be summarized.

Spark Plasma Sintering of Next Generation Nuclear Materials: Daniel Osterberg[1]; Jeff Perkins[1]; Matt Luke[1]; Brian Jaques[1]; Michael Hurley[1]; Darryl Butt[1]; [1]Boise State University

Spark plasma sintering (SPS) has been employed in various materials systems as a novel consolidation method for nuclear materials. SPS has recently seen a broad range of applications and it is considered a potential efficient and cost effective alternative to traditional consolidation methods. Use of SPS for oxide and nitride nuclear fuel fabrication, high level waste reprocessing, radioisotope heat sources, and powder metallurgy has been investigated. Specific materials of interest include Uranium oxide and nitrides, Tungsten cermets, and Nickel alloys.

Step-Wise Exothermic Reactions in Cold-Rolled Ni/Al, Ti/Al, and Ta/Al Multilayer Foils: *Laszlo Kecskes*[1]; Anthony Roberts[1]; Nathan Wingate[1]; Bradley Klotz[2]; Xiaotun Qiu[3]; Jiaping Wang[4]; [1]US Army Research Laboratory; [2]Dynamic Science Inc; [3]Arizona State University; [4]Tsinghua University

Exothermic reactions in cold-rolled Ni/Al, Ti/Al, and Ta/Al reactive multilayer foils were investigated. To understand conditions approaching combustion synthesis reactions, the cold-rolled samples were heated to temperatures above 1000°C in a differential scanning calorimeter. During heating, a series of endo- or exothermic peaks were noted; corresponding to a multi-step process, the relative positions, widths, and amplitudes of the peaks were found to be indicative of a stepwise reaction. Subsequent to obtaining the total calorimetric heat output for a given heating rate, samples were also heated to each peak temperature to identify the intermediate reaction product and evolution of the microstructure from reactants to steady state products. Scanning electron microscopy showed that lower temperature peaks corresponded to aluminum-rich intermetallics, while higher temperature peaks corresponded to conversion of these intermetallics to the nominal composition. Differences in the stepwise reaction mechanisms, as dictated by the underlying intermixing processes, are described.

Structural and Magnetic Properties of Nanocrystalline Fe–Si–Ni Powders Produced by Mechanical Alloying: *Maryam Yazdanmehr*[1]; [1]Technical University of Delft (TuDelft)

Structural and magnetic properties of nanocrystalline Fe–Si–Ni powders produced by mechanical alloying have been studied. The samples with different chemical compositions and milling times were characterized by X-ray diffraction (XRD) and scanning electron microscope (SEM). The alloy powders with average grain size 8–19 nm were synthesized by milling for 35–100 h. Increasing the mechanical alloying time results in the decreasing of both Coercivity and crystallite size. Maximum saturation magnetization and minimum coercivity were obtained at the composition of Fe85Si10Ni5 after 70 h milling.

Structural and Morphological Characterization of Composites of Nylon 6/Ferrite NiFe2O4.: daniella bezerra[1]; Patricia Costa Fernandes[1]; Taciana Regina De Gouveia[1]; edcleide Maria araujo[1]; Ana Cristina Figueiredo Melo Costa[1]; [1]UFCG

In this work, summed up powder NiFe2O4 by the combustion reaction, which was added to a thermoplastic polymer (nylon 6) in order to obtain a composite. The powder was characterized by XRD, nitrogen adsorption by BET and SEM. The ferrite powder was incorporated into the polymer matrix of nylon 6, using a Haake internal mixer Blücher at a temperature of 240°C and 60rpm in concentrations of 30 and 60wt%. The composites of nylon 6/NiFe2O4 were characterized by: XRD and SEM. At both concentrations observed characteristic diffraction peaks of the ferrite and nylon 6. The morphology of composites show that the concentration of 60% of NiFe2O4 showed more clusters and large pores, which was expected due to higher amount of particles. The concentration of 30%, the particles are dispersed, leading to formation of clusters, but smaller than for the composites with concentration of 60%.

Structure and Thermal Oxidation Properties of RuAl and Ru-Al-Ti Alloys Prepared by Mechanical Alloying: *Marlène Clisson*[1]; Julie Gaudet[1]; Lionel Roué[1]; Daniel Guay[1]; [1]INRS

RuAl remain amongst the most efficient materials for high temperature applications in aggressive environments. In this study, nanocrystalline RuAl was prepared by ball milling from elemental Al and Ru powders using both steel and WC crucible and balls. In both cases, RuAl is formed (B2 structure) and pollution by Fe and WC increases with milling time. In the case of pollution by Fe, these atoms are dissolved in the cubic structure of RuAl, while a composite is formed in the case of WC. Thermal gravimetric analysis under pure O2 atmosphere shows that oxidation of RuAl(Fe) is initiated at 380°C. In comparison, the oxidation of RuAl prepared with WC crucible (1 at.% WC) starts at 465°C. The addition of 5 at.% WC to the initial Ru + Al powder mixture yields to a composite whose oxidation is not initiated before 494°C. The origin of this effect will be discussed.

Study of Metal-Oxide Composites Prepared by Ball Milling and Evaluated as Inert Anodes for Aluminum Production: *Sébastien Helle*[1]; Boyd Davis[2]; Daniel Guay[1]; Lionel Roue[1]; [1]INRS EMT; [2]Kingston Process Metallurgy Inc.

In a previous study, we have shown that monophased CuxNi85-xFe15 alloys can be synthesized by high energy ball milling. Alloys with 60<x<85 gave stable potential at 0.5 A/cm2 during 20h of electrolysis in low temperature (700°C) KF-AlF3 electrolyte. The best result in terms of aluminum purity (0.2wt.% Cu) was obtained for the Cu65Ni20Fe15. In this study, further work was performed to improve the corrosion resistance of the electrode and the purity of the produced aluminium. For that purpose, small amount (5 and 15wt.%) of various oxides (Cu2O, CuAlO2, CuAl2O4) were added to pre-milled Cu65Ni20Fe15 to prepare a composite. To achieve this, CuAlO2 and CuAl2O4 were first prepared by mixing copper oxide and alumina via ball milling and heating the resulting material to initiate the reaction. The oxidation at 700°C of the composites was studied and compared to the metal. Finally, 20h aluminium electrolysis tests were conduced in low-temperature KF-AlF3 electrolyte.

Study on Magnetic-Gravity Combination Separation and Acid Leaching of a High Phosphorus Fine Hematite: *Tao Jiang*[1]; Lin Yang[1]; Yufeng Guo[1]; [1]Central South University

Process mineralogy of an Inner Mongolia iron ore was investigated. The results indicated that the iron ore mainly included hematite, a few magnetite and limonite,and the gangues mainly were quartz, secondly Montmorillonite, Spessartite and so on. The dissemination size of primary valuable minerals was fine and uneven distribution . In this work, a method was developed to solve the problem of low recovery of magnetic-gravity separation combined process. An iron concentrate with 61.18% Fe grade and 65.84% recovery could be obtained by low-intensity magnetic separation-High-intensity separation-screening classification-gravity separation combined process. However, the content of phosphorus was highly to 0.510%. The iron concentrate was leached by acid to remove the phosphorus, the content of phosphorus of final iron concentrate was decreased to 0.117%. The iron grade of leached concentrate was increased to 62.93% and total iron recovery of that was reached 64.16%.

Study on Visible Light Photocatalytic Performance of Nano Tungsten Trioxide: *Wu Daoxin*[1]; [1]Changsha University of Science and Technology

Photocatalytic technology is a new environment for energy technology, it has low energy consumption, simple operation, mild reaction conditions, reducing the secondary pollution, etc., and get more and more attention. And tungsten trioxide is an important photocatalytic material, its band gap energy of 3.2eV, less than 500 nm can absorb sunlight. Tungsten trioxide thin films are widely used in electrochromic, solar energy conversion and degradation of pollutants. In this paper, sodium tungstate as raw materials, was used to get tungsten trioxide with nano-sol synthesis. tungsten trioxide samples were charactered XRD (X-ray diffraction), DRS (diffuse reflectance UV-Vis), FS (fluorescent). methyl orange degradation products as the goal, with in the visible light conditions, nano-three-oxide photocatalytic properties were studied, The results show that with the sol-method,tungsten trioxide carried out on methyl orange photocatalytic read its absorbance. It has been showed that the Nano tungsten trioxide has been better properties in the visible band.

Surface Treatment of Materials by Low Energy High Current Pulsed Electron Beam under Evaporating Mode: *Kemin Zhang*[1]; [1]Shanghai University of Engineering Science

The interaction of Low energy high current pulsed electron beam (LEHCPEB) with materials has recently received enormous attention for surface treatment. The LEHCPEB irradiation induces dynamic temperature fields in the surface of the treated materials, giving rise to superfast heating, melting and even evaporating followed by rapid solidification. In the present contribution, the potential of the technique for structure and composition modifications associated with the use of the pulsed electron beam under "evaporating" condition are highlighted. It is shown that the LEHCPEB induced evaporation accounts for the formation of special surface morphology and composition modifications in the treated materials. As a result of these modifications, the corrosion resistance of the treated materials can be significantly improved.

Synthesis of Ag/ZnO Nanocomposite Particles by Ultrasonic Spray Pyrolysis Method: *Sebahattin Gurmen*[1]; Burcak Ebin[1]; [1]Istanbul Technical University

Ag/ZnO nanocomposites have drawn interest because Ag and ZnO are extremely attractive materials to be investigated at the nanoscale due to size- and shape-dependent catalytic, antibacterial, optical and electrical properties which promising various applications for both of them. Combination of their features in nanometer size possesses unique properties and, therefore, offers new technologies and business opportunities. In this research, Ag/ZnO nanocomposite particles were prepared by ultrasonic spray pyrolysis (USP) method using silver nitrate and zinc nitrate aqueous solution in desired concentration under constant air flow rate at 800°C furnace temperature. Then samples were structurally characterized by X-ray diffraction (XRD), scanning electron microscope (SEM) and energy dispersive spectroscopy (EDS). The results show that Ag/ZnO nanocomposite particles in spherical morphology were obtained successfully. Also, it was observed that nanocrystal size of Ag and ZnO in the nanocomposite particles are nearly 36 and 34 nm, respectively which are calculated by Scherrer equation.

Synthesis of Nanostructured Materials for High-Voltage, High-Energy-Capacity Cathode of Li-Ion Batteries: Chunhu Tan[1]; Bob Liu[1]; *Timothy Lin*[1]; [1]Aegis Technology Inc.

There is a great interest in developing energy storage systems based on more advanced lithium ion battery technology. One of the key technologies of such Li-ion batteries is the more advanced cathode material with properties like high energy capacity, good cyclability, enhanced safety and low cost. This presentation is on the development of a novel class of LiMPO4/C (M = Co, Fe) nanocomposite for high-performance cathodes aimed to provide high voltage, high capacity, high charging/discharging rate, excellent stability and low cost. With the support from one ongoing DoE SBIR project, Aegis has established the capability in development and large scale production of advanced electrode materials for high performance Li-ion batteries. The latest results including the establishment of a cost-effective, scalable synthesis process, the influence of key processing parameters on the morphology and sizes of the resultant LiMPO4 particles, and electrochemical tests will be presented.

Temperature and Stress Effects on Cathodic Hydrogen Charging of High-Strength Line-Pipe Steels: *John Roubidoux*[1]; F.J. Sanchez[1]; B. Mishra[1]; D.L. Olson[1]; [1]Colorado School of Mines

The effects of temperature and stress(strain)on cathodic hydrogen charging of high-strength line-pipe steels(X52,X70,and X80)in the presence of a strong and uniform magnetic field will be described.It was experimentally demonstrated that the diffusible hydrogen content in steel is strongly influenced by magnetic induction. The room temperature measurements present both enhanced hydrogen ingress,as well as pitting and cracking behavior. This observation suggests both cathodic and anodic involvement in the magnetocorrosion situation. The elevated temperature experiments were performed to report rate coefficients and apply activated complex theory these electrochemical results. To test the effects of stress on cathodic hydrogen charging of high-strength line-pipe steels,hydrogen charged tensile samples were strained with and without a magnetic field. These observations may have significant implication to hydrogen-cracking susceptibility from magnetic remenance resulting from Magnetic Flux Leakage(MFL) pigging operations on higher strength line pipe steels. These results will be discussed and a comprehensive model will be presented to offer more insight into this behavior.

Temporal Evolution of A Ni-Al-Cr Superalloy with a Dilute Ruthenium Addition: *Yang Zhou*[1]; Dieter Isheim[1]; Gillian Hsieh[1]; David Seidman[1]; [1]Northwestern University

The temporal evolution of a Ni-10.0 Al-8.5 Cr-2.0 Ru at.% alloy aged at 1073 K is investigated using transmission electron microscopy and atom-probe tomography. The gamma-prime-precipitate morphology is spheroidal until 256 h of aging, which is attributed to the Ru addition. The temporal evolution of the gamma-prime-precipitate average radius, volume fraction and number density was investigated and compared to the predictions of classical coarsening models. Contrary to the common belief that refractory additions decelerate the coarsening kinetics, the addition of Ru accelerates the concentration evolution of the gamma-prime- and gamma- phases, which achieve equilibrium values after 0.25 h. The Ru decreases the partitioning of Ni, while increasing the partitioning of Al and Cr at long times. Ruthenium is also responsible for accelerating the partitioning of Ni, Al and Cr. The interfacial width of the gamma-prime/gamma interface is different for each alloying element.

Tensile Deformation Behavior of Zr-Based Bulk Metallic Glass Composite with Different Strain Rate: Kyu-Sik Kim[1]; Ji-Sik Kim[2]; Hoon Huh[3]; *Kee-Ahn Lee*[4]; [1]Center for Advanced Green Materials Technology, Andong National University; [2]Department of Advanced Materials Science and Engineering, Kyungpook National University; [3]Department of Mechanical Engineering, KAIST; [4]Advanced Materials Science and Engineering, Andong National University

Tensile deformation behavior with different strain rate was investigated. $Zr_{56.2}Ti_{13.8}Nb_{5.0}Cu_{6.9}Ni_{5.6}Be_{12.5}$ (bulk metallic glass composite possessed crystal phase which was called ß-phase, dendrite shape, mean size of 20~30µm and occupied 25% of the total volume) was used in this study. Maximum tensile strength was obtained as 1.74GPa at strain rate 10^2 s^{-1} and minimum strength was found to be 1.6GPa at 10^{-1} s^{-1}. And then, maximum plastic deformation showed narrow width local plastic deformation at the strain rate of $5x10^{-2}$ s^{-1} and represented 1.75%, though minimum plastic deformation showed 0%. In the specific range of strain rate, relatively higher plastic deformation and lower ultimate tensile strength were found with lots of shear bands. The fractographical observation after tensile test indicated that wide range of vein like pattern on the fracture surface was well developed especially in the above range of strain rate.

Tensile Failure Analysis of Railway Steels Using Infrared Thermography NDE Technique: *Jeongguk Kim*[1]; Sung Cheol Yoon[1]; Sung-Tae Kwon[1]; [1]Korea Railroad Research Institute

Several different types of railway steels, which are employed for railway vehicle parts such as wheel axle, bogie frame, bolster, and coupler, were introduced to characterize the tensile properties. The tensile specimens were prepared from the actual railway vehicle parts, which were used for over 20 years. During the tensile testing, an infrared camera was used to monitor damage evolution in terms of surface temperature measurements. A qualitative image analysis was conducted to explain failure mode and mechanisms in different railway steel samples based on infrared thermographic images obtained during tensile testing. Moreover, the microstructural characterization using scanning electron microscope (SEM) was performed to correlate the mechanical failure mode with thermographic results. The SEM characterization results were comparable with in-situ monitored IR camera analysis results.

The Effect of Different Heat Treatment Cycles on Controlled Surface Graphitization in CK45 Steel: *Ali-Reza Kiani-Rashid*[1]; Yaser Hamedi[2]; [1]Ferdowsi University of Mashhad; [2]Sharif University of Technology, Tehran

Controlled graphitization has become known as a practical method for improvement of wear resistance and machining properties in steels. In this paper, the effect of heat treatment on microstructure of Ck45 steel has been investigated. Austenitising was carried out at 920°C for 5 hours. Besides, isothermal transformation was conducted at 750°C in the time range of 1-20 hours. The microstructure of the steel considerably changes by this heat treatment process which exhibits the effects of temperature, appropriate austenitising duration and isothermal transformation. Conducted experiments show a suitable distribution of semi-spherical graphite particles especially on the surface of the steel. Also, analyses demonstrate that the amount of formed graphite in the austenitising temperature 920°C is more than graphite in single heat treatment temperature of 750°C.

The Effect of Calcium on Preventing Grain Growth of Al-Zn-Mg Aluminium Alloy: *Sung Yong Shim*[1]; Dae Hwan Kim[1]; Yeong Hwa Kim[1]; In Sang Jeong[1]; In Shup Ahn[1]; Su Gun Lim[1]; [1]K-MEM R&D Cluster, i-Cube Center, Gyeongsang National University

In order to preventing coarsened grain during reheating treatment of thixo-forming process, the effect of calcium on coarsening grain of Al-Zn-Mg Al alloy in the reheating process was investigated. When calcium was added in aluminum alloy, the formed Al_4Ca phase performed grain-boundary pinning, which enabled the reheating process for Thixo-forming to reduce grain growth. In this present, Al-Zn-Mg Al alloys contained calcium (0.3, 0.5 and 0.8 mass %) were fabricated and their microstructures with increasing holding time were observed by optical microscope and scanning electron microscope. The reheating temperature considered as liquid fraction of 10 and 20% was selected by differential thermal analysis and we examined reheating behavior at 600 and 615°. Increasing holding time, the grain growth was inhibited in all alloys except calcium free alloy. What's clear is that calcium contents are able to effectively form fine and equiaxed grain via reheating process at desired temperatures.

The Effect of Frequency of Microarc Oxidation on Surface Properties of 7075 Aluminum Alloys: *Serkan Bozkus*[1]; Murat Baydogan[1]; Huseyin Cimenoglu[1]; Sabri Kayali[1]; [1]Istanbul Technical University

In this study, thick ceramic coatings were fabricated by microarc oxidation on 7075 aluminumalloy in a KOH, Na2SiO3 solution. Micro arc oxidation was performed by using an AC power supply operating in variable frequency between 100 Hz - 167 Hz. Mechanical and physical properties were examined on the surface of the oxide film including hardness, wear resistance and surface roughness. Rockwell C testing was used to compare the relative adhesion characteristics of the oxide film. The unlubricated tribological performance of the coatings was examined using wear system with recipirocating motion against sintered Al2O3 ball. The surface morphology and structure was examined by SEM and X-ray diffractometer. The studied properties of the samples as a function of frequency were discussed.

The Effect of Polymer Structures, Nanoparticle Loadings and Nanoparticle Surface Treatment on the Dynamic Shear Rheological Behaviors of PolydimethylSiloxane (PDMS): *Atarsingh Yadav*[1]; Sameer Pallavkar[1]; Thomas Ho[1]; John Zhanhu Guo[1]; [1]Lamar University

Rheological study of two different types of polydimethylsiloxane (PDMS), low molecular weight (4200, hydroxy terminated) and high molecular weight (139,000, trimethyl siloxy terminated), was investigated under certain range of shear rates to illustrate the viscosity and shear stress variations as a function of shear rate. The shear rate for LMW is 0.1 s-1 to 1200 s-1 and 0.1 s-1 to 200 s-1 for HMW. The investigation was carried out at different temperatures (25°C, 50°C and 70°C). The nanoparticle surface adsorption was used to interpret the observed rheological behavior phenomenon. The effect of Fe2O3 nanoparticle loading and surface treatment with surfactants such as LMW PDMS and oleic acid on the rheological behaviors of PDMS will be presented in this presentation.

The Effects of Nickel in Oxide Layers on the AZ91 Mg Alloys Synthesized by Plasma Electrolytic Oxidation: Dong H. Shin[1]; Ki R. Shin[1]; In J. Hwang[1]; Dong H. Lee[1]; Bongyoung Yoo[1]; [1]Hanyang University

Recently, adding metal ions into electrolyte for plasma electrolytic oxidation(PEO) process to improve the functionality of passivation layer has been widely researched. In this study, Ni ions was incorporated into electrolytes in PEO process, by which the corrosion resistance was enhanced. In addition, the color could be changed from conventional gray to dark brown color, which could be one of the option to improve the appearance of Mg alloy when it is used as a housing of electrical applications. It is also observed that the growth rate of oxide layer increased by nickel ion in electrolyte, and the content of Ni in oxide layer was confirmed as 7.4 at.% when ~350 V was applied.

The Estimation of the Characteristic of Trivalent Chromium Coated Layer According to the Plating Conditions: *Beomsuck Han*[1]; Siyoung Sung[1]; [1]Korea Automotive Technology Institute

The Directive on the restriction of the use of certain hazardous substances(RoHS) in electrical and electronic equipment was adopted by the European Union. This directive restricts the use of six hazardous materials in the manufacture of various types of electronic and electrical equipment. Hexavalent chromium is a main substance of regulated element. Trivalent chromium baths have environmental and health advantages. We are developing a functional trivalent chromium plating bath using a chromium chloride as a replacement for commercial hexavalent chromium plating bath. We make an estimation of the characteristic of coated layer according to the each plating condition using a commercial software(Plating Master). We confirm the characteristic of the practice coated layer.

The Structure Dependence of Rolling Contact Fatigue Damage around Small Cracks for Tempered Martensitic Steel by Electron Backscatter Diffraction Analysis: *Satoshi Morooka*[1]; Yutaka Yamaji[1]; Osamu Umezawa[1]; [1]Yokohama National University

Electron backscatter diffraction (EBSD) analysis has been employed to study local deformation gradient resulted from rolling contact fatigue on a SCM420H martensitic steel tempered at 723K. The fatigue tests were carried out for the specimens involving an artificial hole. The highest damaged region was developed in the specimen interior of about 100 micrometer in depth, where some grains rotated along <111> axis. Cracks were found beneath the region produced in which strain gradient was developed. Misorientation typically near grain boundary were detected in the region and resulted in the localized strain incompatibility near grain boundary. Severe localized plastic deformation at crack-tip may cause dynamic recrystallized fine grains along cracks.

Thermal Oxidation of Titanium Wires: *Tanmay Engineer*[1]; Adriel Apter[1]; Michael Hurley[1]; Darryl Butt[1]; [1]Boise State University

With the objective of growing TiO_2 micro and nanotubes using thermal treatments, the oxidation behavior of pure titanium wires (100 to 2000 μm) was investigated from 800-1200°C in both ambient air, and Ar-20%O_2. In order to derive an oxidation kinetics model for cylindrical geometry, oxide thickness, phase distribution, and morphology were assessed as a function of time and temperature. At higher temperatures, the oxidation mechanism was observed to be complex with larger diameter wires showing formation of distinguishable multilayers of different Ti oxides. The smaller diameter wires formed tubular structures with a compact outer-oxide layer and a porous oxide core. The oxidation rate was observed to be higher in air than that in Ar-20%O_2. At lower temperatures, a thin monolayer of TiO_2 over alpha-Ti core was observed. In conjunction with micro-structural characterization and dimensional measurements, platinum marker experiments were carried out to illustrate the mechanisms of oxidation.

Thermal Tensioning during Welding of DP600 Steel Plates: *Amir Masoud Akbari Pazooki*[1]; [1]TU Delft

Welding often results in a combination of different deformation modes. Thermal tensioning describes a group of techniques to redistribute welding induced residual stresses and thereby mitigate distortion . In this paper a review is given of systems applied in practice. The second part of the paper focuses on Transient Thermal Tensioning by means of additional heating sources attached to the welding torch. Although the technique is already applied in practice, the physical background is not yet fully understood and there is potential for improvement and optimization. In this paper experimental and simulation results of transient thermal tensioning during welding of DP600 steel plates are presented and compared. The influence of process parameters such as the power of the heaters and the position of the heaters with respect to the weld centre line and the welding torch on the final residual stress pattern is also discussed.

Three Dimensional Carbon Nanotube Photovoltaics: *Jack Flicker*[1]; Jud Ready[2]; [1]Georgia Insitute of Technology; [2]Georgia Tech Research Institute

Although photovoltaic technology has been around for over fifty years, the use of a nanostructured, three dimensional morphology in these types of devices has occurred only relatively recently. We introduce a three dimensional photovoltaic device with carbon nanotube pillars coated with photoactive materials to create a solar cell. The extra dimensionality of this cell added by the nanotubes has been theorized to increase the relative energy generated over planar cells by up to four times. The energy increase is due to an increase in the interactions between photons and the photoactive material as the sun is at an off normal angle to the cell substrate. Prototypes of these cells have been made and, although suffering from a low overall efficiency, do show an increased energy production in the same manner that theory predicts when the light source is at an off normal angle.

Thermographic Detection of Artificial Flaws in Polymer Matrix Composite Panel: *Jeongguk Kim*[1]; Sung Cheol Yoon[1]; Jung-Seok Kim[1]; Hyuk-Jin Yoon[1]; [1]Korea Railroad Research Institute

The thermographic detection of artificial flaws on epoxy polymer matrix composites (PMCs) was performed using the infrared thermography method with a high-speed infrared camera. The pulsed thermography with flash lamp was used for the integrity evaluation of PMC panel. The spherical artificial flaws with different diameters and depths were prepared from the panel of glass fiber reinforced epoxy polymer matrix composites. In this investigation, the pulsed thermography was employed to develop a nondestructive evaluation tool for the detection of flaws in PMC panel.

Transient Oxidation and Grain Boundary Characteristics: *Jingxi Zhu*[1]; Laura Fernandez Diaz[1]; Gordon Holcomb[2]; Paul Jablonski[2]; Christopher Cowen[2]; David Laughlin[1]; Sridhar Seetharaman[1]; [1]Carnegie Mellon University; [2]National Energy Technology Laboratory

Oxide ridges were observed to form during the transient stage oxidation of the scale evolution in iron alloys containing 22 wt% Cr that have been held at 800°C in dry air. The post-oxidation characterization through DualBeam® system (focus ion beam and electron beam) combined with 3D reconstruction revealed that the oxide ridges formed on top of the Cr-oxide scale overlapped the intersections of the underlying alloy-grain boundaries with the Cr-oxide scale. Combining the alloy grain boundary characteristics extracted from orientation imaging with SEM characterization, it is found that ridges differ in size with different underlying grain boundaries of different disorientation, which suggests that there is a correlation between the grain boundary diffusivity and grain boundary characteristics.

Transient Thermal Tensioning during Welding of AISI 316L and DP600 Steel Sheets: *Amir Masoud Akbari Pazooki*[1]; [1]TU Delft

Thermal tensioning describes a group of techniques to redistribute welding induced residual stresses and thereby mitigate distortion. In these techniques, different cooling or heating strategies are applied during welding. In this paper experimental and simulation results of transient thermal tensioning during welding of stainless steel (AISI 316L) and dual phase steel (DP 600) are presented and compared. For the numerical simulation Finite Element Analysis 3-D models and extended bar-models have been developed. The influence of process parameters such as the power of the heaters and the position of the heaters with respect to the weld centre line and the welding torch on the final residual stress pattern is also discussed.

Transition Metal Oxide-Doped BaTiO3 Thin Films Prepared by R.F. Magnetron Sputtering: *W. Z. Chang*[1]; J. P. Chu[1]; S. F. Wang[2]; C. H. Wu[1]; [1]National Taiwan University of Science and Technology; [2]National Taipei University of Technology

The perovskite phase BaTiO3 (BTO) is a promising candidate for use as a dielectric in next-generation dynamic random access memory (DRAM) due to its numerous good properties. This presentation reports the effects of transition metal oxide (TMO)-doped BTO thin films with thickness of ~200nm fabricated by r.f. magnetron sputtering on Pt (130nm)/Ti (70nm)/SiO2 (200nm)/Si substrate. Eventually, the metal-insulate-metal (MIM) structure is post-annealing at temperatures up to 650C. The dielectric constants of pure and doped BTO thin films are found to increase with increasing annealing temperature, while they decrease with increasing TMO content. The TMO dopant is also effective to reduce leakage current compared to the pure BTO. This may be attributed to the substitution of cation of TMO in the B site of BTO lattice which might have behaved as the electron acceptor to prevent electrons to pass through.

Twinning during the Tensile Deformation of a TWIP Steel: *Yongfeng Shen*[1]; Yandong Wang[2]; Liang Zuo[3]; Xin Sun[1]; R. Lin Peng[4]; [1]Pacific Northwest National Lab; [2]School of Materials Science and Engineering Beijing Insitute of Technology; [3]Key Laboratory for Anisotropy and Texture of Materials (Ministry of Education), Northeastern University; [4]Department of Mechanical Engineering, Linkoping University

The twinning process and deformation mechanism were investigated by both in-situ tensile test using the synchrotron-based high energy X-ray diffraction (HEXRD) and postmortem TEM observations for a hot-rolled TWIP steel (Fe-20Mn-3Si-3Al). The results clearly showed that the twinning process occurred during the tensile deformation, leading to an increase amount of special grain boundary and optimization of grain boundary structure. The twinning process was facilitated by the crystal with a misorientation of {111}, {222}, {220} and {311}. Interactions between twin boundary and dislocation as well as twin boundary were responsible for the strain hardening during tensile testing. The interactions between primary twins and secondary twins resulted in an additional hardening, enhanced the plasticity in the later stage of deformation. The present strain value of 38% is still less than that of conventional counterpart, which can be due to the fine grain size (~ 5 µm) in the as-prepared specimen.

Water Modeling Study on the Behavior of Inclusions in a Gas-Stirred Ladle with Two Tuyere: *Shu-guo Zheng*[1]; Xiang-yang Chen[1]; Jian-dong Hu[1]; Miao-yong Zhu[1]; [1]Northeastern University

The effects of time, flowrate and mode of gas bubbling on inclusion removal in a 140 ton gas-stirred ladle with two tuyeres were investigated by choosing emulsion drops simulated as inclusions in a water model, and the effect of argon blowing by one tuyere and two tuyere on the inclusion removal was also studied. The results show that most of the inclusions can be removed within eight minutes and all the inclusions which had the possibility to be removed almost disappeared from the system in twenty-eight minutes. There was both an optimal gas flowrate for the inclusion removal with the high and the low gas flowrates, which was explained by discussing the mechanism of inclusion removal. Argon blowing by one tuyere seemed to be more efficient for inclusion removal within six minutes gas blowing than argon blowing by two tuyeres, in contrast, in the further course of blowing, argon blowing by two tuyeres were more efficient. The mode of gas bubbling with firstly larger gas flowrate and then smaller flowrate seemed to be efficient for inclusions removal. Furthermore, it had been found that the inclusion removal was in exponential relationship with gas blowing time.