2009 Functional and Structural Nanomaterials: Fabrication, Properties, and Applications: Nanoscale Powders: Materials, Synthesis and Applications

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Nanomaterials Committee, TMS: Nanomechanical Materials Behavior Committee

Program Organizers: Gregory Thompson, University of Alabama; Amit Misra, Los Alamos National Laboratory; David Stollberg, Georgia Tech Research Institute; Jiyoung Kim, University of Texas at Dallas; Seong Jin Koh, University of Texas at Arlington; Wonbong Choi, Florida International University; Alexander Howard, Air Force Research Laboratory

Thursday AM — Room: 3018
February 19, 2009 — Location: Moscone West Convention Center

Session Chair: Gregory Thompson, University of Alabama

8:30 AM

Mono-Dispersed Nano-Crystalline Aggregated Nickel Powders Obtained by Using Hydrazine in the Presence of Sodium Dodecyl Sulphate: *Mohammad Hussain*[1]; [1]KACST

A range of aggregated mono-dispersed nano-crystalline nickel powders has been synthesized by chemical reduction process using hydrazine as a reducing agent at 600C. The rate of reaction was further accelerated as the temperature was increased to 800C. Under reflux conditions at 1000C, the rate of reaction was much faster and even finer powders were obtained. The aggregated powders were characterized by XRD, SEM and TEM. The results showed the presence of nickel particles which were less than 20nm in diameter. The particle size of the synthesized metal powders was also measured at room temperature (RT) using Nano ZS Particle Sizer instrument (Malvern Instrument), which utilizes the technique of dynamic light scattering (DLS). Further thermodynamic measurements were carried out using Differential Scanning Calorimeter (DSC) and Thermal Gravimetric Analyser (TGA) to establish any differences in the energy levels of the powders synthesized by different methods. These results are further discussed.

8:45 AM

Nano-Powders of Ni_3N and Ni Metal Prepared through Liquid Ammonia Solution: Zhao Han[1]; *Hailong Qiu*[1]; Hongmin Zhu[1]; [1]Beijing University of Science and Technology

Nickel nitride(Ni_3N) nano-powders were synthesized through chemical reduction, of $NiCl_2$ by sodium in liquid ammonia at -45°C. The produced Ni_3N nano-powders were heat-treated and subsequently converted to nickel metal nano-powders at 300°C. The crystal structures and particle morphologies of the products were characterized by X-ray powder diffraction(XRD) and field emission scanning electron microscope(SEM). The results indicated that the products were hexagonal Ni_3N and cubic nickel metal powders, with average particle size of 21 nm and 19 nm, respectively. The possible mechanisms of the reactions were also discussed.

9:00 AM

Consolidation of Gas Atomized Precursor Alloy Powder for the Formation of an Oxide Dispersion Strengthened Ferritic Stainless Steel Microstructure: *Joel Rieken*[1]; I. Anderson[2]; M. Kramer[2]; Y. Wu[2]; J. Anderegg[2]; [1]Iowa State University; [2]Ames Laboratory

Gas atomization reaction synthesis (GARS) was used as an innovative route for the fabrication of precursor oxide dispersion strengthened ferritic stainless steel powder. During this process the as-atomized powder particles, with a nominal chemical composition of Fe-(12.5-15.0)Cr-(0.5-1.0)Y-(0.0-0.54)Ti-(0.0-3.0)W wt.%, were reacted in situ forming a thin surface oxide. The surface oxide of the particles is intended to act as an internal oxygen supply reservoir for the formation of nano-metric yttrium-enriched oxide dispersoids. The formation of the nano-metric dispersoids occurs during elevated temperature consolidation of the powders and is driven by an oxygen exchange reaction between the initial surface oxide (e.g., chromium oxide) and yttrium metal. Microstructure phase evaluation was performed using scanning electron microscopy and transmission electron microscopy. Elevated temperature tensile testing was used to examine the initial strength of the as-consolidated specimens. Support from the DOE-FE (ARM program) through Ames Laboratory contract no. DE-AC02-07CH11358 is gratefully acknowledged.

9:15 AM

Synthesis of Nano-Scale Fibrous Ni/Co Alloy Powders from Complex Nickel-Cobalt Oxalate Containing Ammonia: Zhan Jing[1]; Zhang Chuanfu[1]; Huang Boyun[1]; He Yuehui[1]; *Fan Youqi*[1]; [1]Central South University

A nickel–cobalt oxalate complex precursor containing ammonium for the synthesis of nano-scale fibrous nickel cobalt powder was obtained by coordination coprecipitation techinique under suitable conditions. The experimental conditions including feeding methods, precipitation temperature, reactant concentration, surfactant, washing method and pH value of solution that influence the morphology, average particle size and the dispersion of the precursor have been studied in detail. SEM, XRD pattern, thermal analysis and IR spectroscopy were used in the characterization and the evaluation of some aspects of the formation mechanism of fibrous morphology of the precursor. The crystallinity, purity, and surface morphology of the as-prepared NixCo1-x fibers were investigated by XRD, SEM, respectively. The X-ray photoelectron spectroscopic(XPS) data have confirmed that the nickel and cobalt in the bimetallic nano-scale fibre are in the zero-valence state.

9:30 AM

Optical and Magnetic Properties of Transition Metal-Doped ZnO Nanoscale Powders Synthesized by Chemical Method: *M. Khan*[1]; [1]Center for Advanced Mathematics and Physics

We report the results of a detailed investigation of sol–gel-synthesized nanoscale (Co,Mn) co-doped ZnO powders processed at 600°C in forming gas (Ar95%+H5%) to understand how the structural, optical and magnetic properties of ZnO are modified by doping, in addition to searching for the theoretically predicted ferromagnetism. X-ray diffraction results indicate a purely single phase. The diffused reflectance spectroscopy revealed many characteristic absorption bands correspond to the Co+2 ions and Mn+2 ions in tetrahedral symmetry, indicating that dopants (Co, Mn) are well substituted in ZnO lattice. Magnetic measurements showed a paramagnetic when the samples annealed in air. However a weak ferromagnetic behaviour was observed for the sample containing Mn (4at%) while Co varied x = 0.00-0.02. One the other hand a relatively strong ferromagnetic coupling observed in the samples containing Co (4at%) with Mn variation. The mechanism of ferromagnetic behavior can be interpreted in light of F-center exchange (FCE) model.

9:45 AM

Synthesis and Crystallization of Amorphous Nano-Sized Si-B-N Powders: *Hailong Qiu*[1]; Mei Yang[1]; Zhao Han[1]; Hongmin Zhu[1]; [1]Beijing University of Science and Technology

Si-B-N ceramic powders were prepared through chemical reduction of $SiCl_4$ and BBr_3 by sodium in liquid ammonia. The products obtained were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), and selected area electron diffraction (SAED). The results indicated that the products were amorphous phase with the particle size less than 50nm. The powders were heat-treated under vacuum at various temperatures. Up to 1500°C, the powder remained in amorphous phase. When the powders were heated at temperatures higher than 1500°C, crystallites of silicon nitride and boron nitride appeared form the matrix phase.

Alumina and Bauxite: Process Improvements and Experiences - White Side

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee
Program Organizers: Everett Phillips, Nalco Co; Sringeri Chandrashekar, Dubai Aluminum Co

Thursday AM Room: 2002
February 19, 2009 Location: Moscone West Convention Center

Session Chair: Carlos Suarez, Hatch Associates Inc

8:30 AM Introductory Comments

8:35 AM
Electrocatalytic Oxidation of Organics in Bayer Liquor: *Anthony Perrotta*[1]; Fred Williams[2]; [1]Pennsylvania State University; [2]CMIS Corp

Electrochemical oxidation for chemical bleaching of wood pulp was developed by the Dow Chemical Company. The present work used the Dow approach to electrochemically oxidize organics in a Kwinana spent liquor by the in situ cathodic reduction of oxygen to peroxide using only air as feed. Significant oxidation of the organics, relative to steel electrodes, was achieved using platinum, and platinum alloyed with 10% rhodium. The TOC reduction showed a decrease from 22g/l to 18g/l, 12g/l, and 7g/l for the steel, platinum, and platinum-10%rhodium electrodes, respectively. The electrocatalytic oxidation, obtained with the Pt-10Rh electrode shows, in accord with enhanced TOC reduction, the sodium carbonate concentration increasing from 50g/l to 150g/l. In comparison, the sodium oxalate concentration remained essentially unchanged. In conclusion, electrocatalytic oxidation is shown to be effective in a spent plant liquor in the presence of liquor impurities.

9:00 AM
The Influence of Moisture in the Attrition Index of Alumina: *Jorge Lima*[1]; Joaquim Ribeiro[1]; Cleto Júnior[1]; Clauderino Batista[1]; [1]ALUNORTE

Attrition index is one of the most important physical parameter to define smelting grade alumina quality. Several papers have been correlated alumina morphology with strength. The present paper has the main objective to investigate the moisture influence in the attrition index measurement and the alumina strength. Alumina has a high capacity to absorb water from the environment, due to high surface area available to water absorption. It is very well know that water content can affect the alumina performance during the pot room operations, i.e. handling, HF control and formation of geysers and volcanoes, but fewer papers make relations between moisture and attrition index or strength. Presently, we discuss the attrition index analytical method, water adsorption and how they correlate each other, using particle size distribution, moisture, LOI and surface area analysis.

9:25 AM
The World's Largest Hydrate Pan Filter: Engineering Improvements and Experiences: *Birger Petersen*[1]; *Manfred Bach*[2]; Rolf Arpe[1]; [1]Aluminium Oxid Stade GmbH; [2]FLSmidth Dorr-Oliver Eimco GmbH

FLSmidth Dorr-Oliver Eimco GmbH (FLS) and Aluminium Oxid Stade GmbH (AOS) present the latest engineering highlights and details of the operation of the world's largest hydrate pan filter at AOS. The various features of the pan filter with a filtration area of 71m² have resulted in AOS's decision to use FLS technology for product filtration. A track record is provided that deals with experiences of the filter operation. This covers the major process features and the operating procedures, which have been developed to maximize the availability and performance of the filtration system. Comments are made concerning a comparison with the operation of hydrate drum filters used before the commissioning of the 71m² pan filter. The production of high quality hydrate is discussed in relation to filtration parameters and optimization measures which have been practiced since the startup of the filter.

9:50 AM Break

10:10 AM
Superior Arguments for Most Modern Filtration Technologies in High Capacity Alumina Refineries: *Reinhard Bott*[1]; Thomas Langeloh[1]; Juergen Hahn[1]; [1]BOKELA GMBH

In the last years capacity of alumina plants steadily increased leading to high capacity alumina refineries with annual production rates up to 3 Mt/y and even more. Before this background requirements on filtration technologies increased and great importance is placed on factors such as performance capacity, improved operation control, availability of equipment, reliability of operation, ease of maintenance or impact of the filtration process on downstream processing. The paper highlights characteristics in the design, construction and operation control of modern filtration technologies which are decisive to meet these increased requirements, by exemplary focusing of backflush filters for polishing filtration and pan filters for product filtration.

10:35 AM
Energy Efficiency in Gas Suspension Calciners (GSC): *Susanne Wind*[1]; Benny Raahauge[1]; [1]FLSmidth Minerals A/S

Since commissioning three 4500 tpd. GSC units, the world's largest calciner installation at Queensland Alumina Limited in 2004, FLSmidth Minerals has introduced it's new generation Gas Suspension Calciner Technology in order to obtain enhanced performance. The new generation Gas Suspension Calciners include the installation of a Fluidised Holding Vessel in the Furnace Cyclone after the Calciner Furnace, now being introduced into several new GSC units under design and construction. In addition to the Holding Vessel, a Forced Draft fan can be added to existing installations to increase capacity and provide enhanced operation. The paper will present the new generation Gas Suspension Calciner from FLSmidth Minerals and will focus on energy efficiency, alumina quality and upgrade possibilities of existing units.

11:00 AM
Increased Availability and Optimization of Calciner Performance Due to Automation: *Michael Missalla*[1]; Jan Jarzembowski[1]; Roger Bligh[1]; Hans-Werner Schmidt[1]; [1]Outotec GmbH

In the last 30 years, Outotec has installed more than 50 calciners worldwide. Over the years the operation was improved significantly and thus also availability was raised. Real costs for instrumentation and control systems have also reduced over this period, thus encouraging the installation of more instrumentation, data analysis and better process monitoring. More recently, the trend has been towards full automation of activities like capacity load changes while maintaining other performance and product quality related parameters within specification. Other examples of improved automation are the use of advanced control loops with multiple input, while preheating and shut down of the calcination plant can be achieved with just the push of a button. The benefits of improved automation include improved availability through avoidance of operator error, reduction in manpower for process control related tasks and reduced requirement for field adjustment in potentially hazardous areas. The implementation of multivariable control strategies in recently commissioned plants and comprehensively engineered control concepts are described. Furnace temperature feed forward control, automated pre-heating, start-up, gas and solids purge, equipment protection monitoring, and automated protective measures for operational stability and plant trip prevention are presented.

11:25 AM Concluding Comments

Aluminum Alloys: Fabrication, Characterization and Applications: Composite and Foam

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Processing Committee
Program Organizers: Weimin Yin, Williams Advanced Materials; Subodh Das, Phinix LLC; Zhengdong Long, Kaiser Aluminum Company

Thursday AM Room: 2004
February 19, 2009 Location: Moscone West Convention Center

Session Chair: Zhengdong Long, Kaiser Aluminum Company

8:30 AM
Joining of Aluminum 5754 Alloy to Carbon Fiber Reinforced Polymers (CFRP) by Ultrasonic Welding: *Frank Balle*[1]; Guntram Wagner[1]; Dietmar Eifler[1]; [1]University of Kaiserslautern, Institute of Materials Science and Engineering, Germany

Ultrasonic metal welds were performed to realize aluminum alloy/carbon fiber reinforced polymer (CFRP) – joints. Important advantages of ultrasonic welding are welding times less then three seconds and welding temperatures below 450°C. Important steps of the process are the softening and displacing of the polymer out of the welding zone by the ultrasonic shear oscillation. In the following, in contrast to conventional joining processes a direct contact between the aluminum surface and the carbon fibers takes place. The bonding mechanisms can be shown in detail by scanning electron microscopy. In a first step shear strengths of about 30 MPa were realized for AA5754/CF-PA66 – joints. By special surface pre-treatments of the metal, for example shot peening or etching, the joint strength could be increased up to 60%. Finally, the cyclic deformation behavior of these hybrid joints and the influence of aging in selected climates will be discussed.

8:50 AM
Study of Particle-Matrix Interaction in Al/AlB2 Composite Material via Nanoindentation: *Zenon Melgarejo*[1]; Pedro Resto[1]; Donald Stone[1]; Marcelo Suárez[2]; [1]University of Wisconsin; [2]University of Puerto Rico-Mayagüez

The tribological performance of functionally graded Al/AlB2 composites produced by centrifugal casting has demonstrated the suitability of these materials for lightweight, high wear resistance components. Hard AlB2 particles embedded in the composites promote wear strength, which is also critically dependent on the Al matrix-particle interaction. To measure AlB2 properties and understand the particle-matrix interaction nanoindentation experiments were performed on 3-10 µm diameter AlB2 particles embedded in the aluminum matrix of an Al-5 wt%B gravity cast alloy. Elastic modulus and hardness were obtained by separating out the effects of the surrounding aluminum matrix. Orientation-dependence of the mechanical properties of the AlB2 particles was assessed using electron backscattered diffraction. Under large nanoindentation loads, AlB2 particles could be pushed into the matrix. On a per-area basis smaller particles were more difficult to push in than larger particles. Strain gradient plasticity theory was used to explain the size dependence of the push-in force.

9:10 AM
Study of Microstructure-Mechanical Properties Relationship in Accumulative Roll Bonding Processed Al6016 Alloy: *Suhash Dey*[1]; Juliane Hüttenrauch[1]; Klemens Reuther[1]; Werner Skrotzki[1]; [1]Technische Universität Dresden

Ultrafine grained (UFG), less than 1 micrometer, metals and alloys provide more strength to the material than coarser grained (more than 1 micrometer). Severe plastic deformation is one way to generate UFG materials and there exists several ways to perform for eg. equal-channel angular extrusion/ pressing, accumulative roll bonding (ARB), high pressure torsion, etc. ARB technique looks promising as one can achieve UFG materials in the form of bulk sheets. ARB is the process which bonds two material surfaces while rolling simultaneously. This is a relatively new technique and requires comprehensive microstructural-textural-mechanical properties studies on different materials. In the conference, ARB performed on AA6016 alloy would be presented with its microstructure-mechanical properties relationship in full details.

9:30 AM
Sintering Response of Aluminum Alloys with and without Addition of Si and SiC By Powder Metallurgy: *Antonyraj Arockiasamy*[1]; Seong J. Park[1]; Randall M. German[2]; Pavan Suri[3]; Paul Wang[1]; [1]Mississippi State University; [2]San Diego State University; [3]Heraeus

The demand for lightweight automotive components from aluminum and its alloys is turning to powder metallurgy (P/M) for optimal combinations of strength and creep, especially when the properties are required beyond that possible from a cast ingot route. This paper describes the die compaction and sintering response of aluminum with and without the addition of Si and SiC. A design of sintering experiments involving three sintering temperatures, hold times, and heating rates based on the Taguchi method was employed to isolate the optimum processing sintering cycle. Besides the mechanical properties, phase transformation and microstructure are investigated using hardness testing, compression-tension testing, dilatometry, thermogravimetric analysis coupled with differential scanning calorimeter and scanning electron microscopy with energy dispersive spectroscopy. A comparison study has also been made to analyze the strength and weakness of sintered aluminum alloys and ranked in terms of the effectiveness of the alloys based on their mechanical properties.

9:50 AM
Impact Properties and Microstructural Evolution of Weldable and Unweldable Aluminum-Scandium (Al-Sc) Alloys: *Woei-Shyan Lee*[1]; Tao-Hsing Chen[1]; [1]National Cheng Kung University

This study employs a compressive split-Hopkinson pressure bar to investigate the impact properties of two weldable and unweldable Al-Sc alloys at strain rates ranging from1.2×103s-1 to 5.9×103s-1 and temperatures of –100°, 25° and 300°, respectively. The results indicate that for both alloys, the impact properties are found to be significantly dependent on both the strain rate and temperature. Moreover, the flow stress, work hardening rate and strain rate sensitivity are higher in the unweldable Al-Sc alloy than in the weldable alloy. In describing the plastic deformation behaviour of the two Al-Sc alloys using the Zerilli-Armstrong fcc constitutive model. The TEM observations reveal that in both alloys, the dislocation density increases with increasing strain rate, but decreasing with increasing temperature. Furthermore, it is found that the dislocation density of the unweldable Al-Sc alloy is higher than that of the weldable Al-Sc alloy.

10:10 AM Break

10:30 AM
An Investigation into the Mechanical Behaviour of 7075-Al Based Composites: *Indumati Deshmanya*[1]; G. K. Purohit[1]; [1]Poojya Doddappa Appa College of Engineering, Gulbarga

Metal matrix composite (MMC) materials are finding applications in various fields ranging from cutting tools to aero-space materials because of their high strength-to-weight ratios, high wear resistance and easy manufacturability. Extensive research work on the feasibility of these composites is undertaken by the authors. A knowledge of their mechanical behaviors is believed to enhance their applicability. This paper presents the results of a study on the mechanical behavior of 7075-AL alloys with AL_2O_3 reinforcing produced by stir casting. Factorial design techniques and ANOVA have been used to develop models. Of these, 7075-Al alloy composites are of particular importance because of their suitability in wear resistant, corrosion resistant and fracture resistant environment hardness and impact strength (Charpy-V) have been performed on specimens, which are carefully extracted from the cast material. The effect of particle size (100m-400m), of reinforcement (5% to 12% by weight), sintering temperature and holding time on the selected mechanical properties are reported. An attempt is made to correlate the results with microstructural studies.

10:50 AM
Effect of Aging on the Mechanical and Corrosion Performance of 7012 Al Matrix SiC Particle Reinforced Composites: Harun Mindivan[1]; Eyup Kayali[2]; *Huseyin Cimenoglu*[2]; [1]Ataturk University; [2]Istanbul Technical University

In this study mechanical and corrosion properties of 7012 aluminum alloy matrix 50 vol.% SiC particle reinforced composites produced with a squeeze casting technique has be examined in as-cast and T6 tempered states. Mechanical properties of the composites were determined by hardness measurements, impact tests and wear tests. Corrosion tests were carried out according to ISO 11846 standard by immersing the composites in a "30g/l NaCl + 10 ml/l HCl" solution for 24 hours. T6 tempering improved the hardness, wear resistance and corrosion resistance while reducing the impact toughness.

11:10 AM

Fabrication Process of Hybrid Porous Structured Aluminum: *Young Ik Seo*[1]; Chang Won Park[1]; Dae-Gun Kim[1]; Kyu Hwan Lee[2]; Young Do Kim[1]; [1]Hanyang University; [2]Korea Institute of Science and Technology

Porous materials can be applied to products with various functions such as energy absorption systems, light weight structures, and air/water filtration systems. Especially, the filtration system using the metallic membrane should have good permeability and excellent filtration efficiency. In this study, a hybrid porous structure was created by styrofoam for macropore network and surface modification for nanoporous surface. A mixture of Al powder, styrofoam and PVP solution was formed in an Al tube and then was dried in oven at 60°C for 1 hour. Styrofoam and binder were removed at 450°C for 2 hours and were subsequently heated up to over 600°C. The fabricated macroporous Al body was surface-modified in dilute alkali solution with different concentrations. The optical microscopy and scanning electron microscopy were employed to investigate the microstructure. The characteristics of pores were confirmed through the porosimeter and Brunauer-Emmett-Teller method.

Aluminum Reduction Technology: Modelling

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee

Program Organizers: Gilles Dufour, Alcoa Canada, Primary Metals; Martin Iffert, Trimet Aluminium AG; Geoffrey Bearne, Rio Tinto Alcan; Jayson Tessier, Alcoa Deschambault

Thursday AM — Room: 2012
February 19, 2009 — Location: Moscone West Convention Center

Session Chairs: Daniel Richard, Hatch Associates Ltd; Marc Dupuis, GeniSim Inc

8:30 AM

Busbar Arrangement Optimization for End Cells: *Donald Ziegler*[1]; Yimin Ruan[1]; [1]Alcoa Inc

Cells at the ends of potrooms have magnetic environments different from those in the rest of the potline. Their lack of close neighbors on one side and the effects of the crossover or rectifier bus can cause these cells to have serious magnetic problems if they are not appropriately compensated. We use examples of this problem to further examine the possibilities of automated optimization of magnetic fields in Hall cells. We discuss an objective function that takes partial account of the effect of the steel in the end cells.

8:50 AM

Heat Transfer Considerations for DC Busbars Sizing: *Andre Schneider*[1]; Tom Plikas[2]; Daniel Richard[1]; Lowy Gunnewiek[2]; [1]Hatch; [2]Hatch, Sheridan Science & Technology Park

The main DC busbars connecting the rectifiers to the potrooms or connecting the potrooms of a potline often consist of several naturally cooled parallel bars. To reduce cost, sizing of the bars is usually based on the minimum bar cross-section at the maximum allowable bar temperature. An adequate representation of the heat transfer characteristics of the bar system is therefore required for an efficient design of both busbars (preventing excessive costs or overheating) and expansion joints. A discussion on radiation and natural convection heat losses of the bars to the ambient is made using detailed Computational Fluid Dynamics (CFD) simulations. The effects of bar geometry, bar-to-bar spacing, ambient conditions and current density are discussed. Finally, a simplified calculation methodology based on semi-empirical convection correlations and analytical radiation view factors is proposed. Potential industrial applications, for example increasing the line amperage of existing potlines, are discussed.

9:10 AM

The Effect of Channel Width under Different Bath Forces on the Aluminium Reduction Cell Current Efficiency: *Mohamed Ali*[1]; Mohamed Doheim[1]; Abdel Fattah El-Kersh[1]; [1]Egyptalum

A two-dimensional mathematical model is used to study the effect of changing channel width on current density, bath circulation and current efficiency. The current density decreases towards the side wall carbon blocks and this is more pronounced as the channel width increases. The gas bubbles induced force is more effective compared with electromagnetic forces (EMFs). The bath velocity values under various driving forces, bubble, EMFs, and the combined effect, were increased with reducing the channel widths. The reduction in channel width by 10 cm for the conditions representing the actual situation of the cell leads to increase the current efficiency by 0.4 %.

9:30 AM

The Impact of Cell Ventilation on the Top Heat Losses and Fugitive Emissions in an Aluminium Smelting Cell: *Haiam Abbas*[1]; Mark Taylor[1]; Mohammed Farid[2]; John Chen[1]; [1]Light Metals Research Center, University of Auckland; [2]Chemical and Materials Engineering, University of Auckland

Problems associated with aluminium smelting cell ventilation, caused by leakage of fume gases through pots superstructure gaps into the potroom, are normally solved by increasing the fume suction rate (draught) above certain levels. It is also known that, fugitive emissions are associated with reducing the draught below certain critical levels. Top heat losses are increasing in smelting cells as line amperage is raised. This drives further fugitive emissions through greater buoyancy of the fume/air mixture. A quantitative understanding of the relationship between fugitive emissions, superstructure tightness, top heat loss, and cell draught is crucial in the environmental context. It is also important if this top heat loss could be recovered for re-use. This problem is studied here computationally using the ANSYS-CFX software. Possibilities to improve cell ventilation and to decrease fugitive emissions are analysed for a typical industrial cell. The computed cell emissions and temperatures are compared with measured values. The impact of draught on ventilation and heat loss is also discussed.

9:50 AM

A Modelling Approach to Estimate Bath and Metal Heat Transfer Coefficients: *Dagoberto Severo*[1]; Vanderlei Gusberti[1]; [1]PCE Ltd

The heat transfer coefficients between the cell cavity and the liquids (bath and metal) are important parameters in order to achieve correct thermal calculations of the electrolytic cell's behavior. Traditionally, the wall heat transfer coefficients are adjusted with help of thermal measurements done in the real existent cells. However, this procedure cannot be done in a new project. The present work aims to show numerical procedures for estimation of the local heat transfer coefficients, at the liquid bath regions, independent of previous measurements. These results can be compared with the values obtained by experimental correlation formulae developed using physical models with similar fluids. The influence of anode-ledge channel width, interanode channels width, anode width, slots and anode immersion depth as well the current density passing through the anodes on heat transfer coefficients are investigated by numerical experiments.

10:10 AM Break

10:30 AM

Comparison of Two Different Numerical Methods for Predicting the Formation of the Side Ledge in an Aluminium Electrolysis Cell: Clement Bertrand[1]; Marc-Andre Marois[1]; *Martin Desilets*[1]; Marcel Lacroix[1]; Marie-Michelle Coulombe[1]; [1]Sherbrooke University

The solid-liquid phase change problem that takes place on the inside walls of an aluminium reduction cell has been modelled using two numerical approaches. In the first approach, called the single phase method, the phase change is not modelled explicitly, i.e., the solidification front is estimated by tuning cleverly the thermophysical properties of the liquid electrolyte. In the second approach, the phase change is modelled with an enthalpy method. In this case, heat transfer in all phases is calculated and the phase change is taken into account via a liquid fraction for the melt. Both methods are tested and compared to a benchmark problem from the literature. In spite of the fact that both methods are fairly robust and accurate for predicting the steady state condition, only the enthalpy method can predict the time-varying shape of the side ledge in situations like the cell cooling during a potline power interruption.

10:50 AM

Solutions for the Metal-Bath Interface in Aluminium Electrolysis Cells: *Valdis Bojarevics*[1]; Koulis Pericleous[1]; [1]University of Greenwich

The dynamic MHD modelling package is applied to the simple test case presented recently by Dagoberto, et al. in Light Metals 2008. It is compared to the derived analytical solution for a variation of boundary conditions. The interface stability is tested and compared to previously published analytical solutions. The problem is extended by a simple busbar design in order to run the universal busbar design tool and to apply it for the dynamic simulations of the electromagnetic fields, the interface waves and the velocity field.

11:10 AM

Fluid Flow and Bubble Behavior in the Aluminum Electrolysis Cell: *Lifeng Zhang*[1]; Yufeng Wang[1]; Xiangjun Zuo[1]; [1]Missouri University of Science and Technology

A full scale water model was established to investigate the phenomena in aluminum reduction cells. The behavior of bubbles under the anode is analyzed by both directly observation and camera recording. Bubble under the anode has a thick bubble front and a thin, long trail portion. With 0o tilted angle, hardly can the bubbles move forward, but form a gas film under the anode. With non-zero tilted angle, bubble motion under the anode is driven by the buoyancy force, thus bubbles are easy to escape through the curved end of the anode. LDV was used to investigate the fluid flow pattern. The LDV measurements reveal a recirculation flow pattern in side channel, similar to the observation of the tracer dispersion. Larger tilted angle and larger gas flow rate generate larger velocity and bigger turbulent energy, especially in the region close to the end of the anode and the top surface.

Aluminum Reduction Technology: Potroom Operation and Maintenance

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee

Program Organizers: Gilles Dufour, Alcoa Canada, Primary Metals; Martin Iffert, Trimet Aluminium AG; Geoffrey Bearne, Rio Tinto Alcan; Jayson Tessier, Alcoa Deschambault

Thursday AM — Room: 2001
February 19, 2009 — Location: Moscone West Convention Center

Session Chair: Michel Reverdy, Dubal

8:30 AM

Alcoa Maintenance Best Practices: To Achieve Excellence in Planning, Scheduling, Autonomous Maintenance and Reliability: *Maurice Beaudry*[1]; Marco Plante[1]; [1]Alcoa-Deschambault Aluminum Smelter

At Alcoa Aluminum smelter in Deschambault, Quebec, planning, scheduling, autonomous maintenance and reliability are already established. This abstract is to show the importance of a good planned maintenance on the production and profit to the plant. How to maintain a high equipment reliability level to improve the client satisfaction to a higher level (production), to reduce our production cost, reduce maint. cost by reducing our unplanned jobs (emergencies) and maintain a good operational availability (oa). Our success is based on our culture and values. In 2002, this Alcoa plant won the North American Maintenance Excellence Award (Name) who is an annual program conducted by the foundation for Industrial maintenance Excellence to recognize North American companies that excell in performing the maintenance process. The program not only covers maintenance,but the entire organizational structure. The main benefit and not the less was to be acknowledged as a world leader in maintenance.

8:50 AM

Reliability and Maintenance Excellence from "Cradle to Grave": *Serge Mathieu*[1]; [1]ABB Inc

Energy costs and metal prices have increased, environmental and safety have become Sr management main concerns. Industry must change the way major projects are delivered. Have you ever, as a production mgr or a maintenance mgr been given a new equipment, a new line or a new plant and been told "Now it is yours, operate and/or maintain it". As production or maintenance managers, yours objectives are to accelerate the start-up and get a sustainable uptime asap. Reliability and Maintenance began at the design phase of a project. This presentation will demonstrate how we can deliver a Reliable project to the production and maintenance manager by integrating the Reliability concepts and the maintenance best practices right at the design phase, through the commissioning and start-up.

9:10 AM

Pure Metal Production and Methodology: The Alcoa Deschambault Experience: *Stephen Lindsay*[1]; Patrice Doiron[2]; [1]Alcoa Primary Metals; [2]Alcoa Deschambault

Since 2005, Alcoa Aluminerie de Deshambeault as kept iron level under 850 ppm. Many tools and trial has been developed and tested to achieve this performance. In this presentation, we will share methodology used, success key item, trial result and best practice that help plant achieve and maintain those result.

9:30 AM

A Simple Method for Alumina Homogenization in Large Silos: Geir Wedde[1]; *Ketil Rye*[2]; Gaute Nyland[2]; [1]Alstom Norway AS; [2]Elkem Aluminium ASA

In many silo systems for the aluminium industry little emphasis was laid on the way the alumina was fed into the silos. Simply one point of entry at center of top of silo was widely used. As the powder drops to the top of the alumina level inside the silo the powder segregates with effects when discharged into downstream systems such as dry scrubbers, alumina transport and pot feeding systems. Sampling of alumina discharged from an enriched alumina silo at the Elkem Mosjoen smelter demonstrated systematic large differences in the fines fraction being fed the pots. Typically, one potroom received twice as much fines as the other. An anti-segregation system was integrated in the silo with a challenge on restricted heights and space. Immediately after connecting up the anti-segregation system sampling of the two alumina discharge spouts consistently demonstrated a homogenous alumina with equal fractions of fines and fluoride content.

9:50 AM

Issues Arising from the Back EMF in Potlines: *Ali Mohamed*[1]; Arvind Kumar[1]; Maryam Al Jallaf[1]; [1]Dubai Aluminium Co Ltd

In a rapidly collapsing line current to zero, the cells are known to have an electrode potential which stays on during zero load situation. It is termed as back electromotive force (back emf). During this period, the cells behave as a battery since anodes have partially discharged intermediates in a thin region on its surface. Back emf decays with time from a high value of ~1.7 to ~1.0 volt. It plays a pivotal role during a power outage period and during power restoration. Safety issues and 'earthing' a potline circuit are of paramount importance when working on cut out pots. This paper covers a study of back emf during planned power outages at DUBAL and work practices evolved as a result to handle such a situation. The paper also covers the importance of deploying a portable 'earth' when working on cut out cells.

10:10 AM Break

10:30 AM

Electrolysis Pots Anode Changing Automation: Impact on Process and Safety Performances: *Nicolas Dupas*[1]; [1]ECL

The anode changing of the electrolysis pots is a recurring procedure in the aluminium smelter. Traditional methods involve a floor operator and a Pot Tending Machine to conduct the task. The precise vertical positioning of the new anode bottom surface with respect to the molten aluminium is critical to the stability of the electrolysis pot, to its overall performance, and therefore to the productivity of the smelter. The anode changing process is a determining factor in the safety and productivity of the potlines. By developing unique technical solutions and implementing a high level of automation in this process, it is possible to not only greatly increase its precision and repeatability, but also to alleviate the associated safety risks for pot floor operators. Such new solutions have been implemented in a renowned North American smelter, allowing a complete study of its benefits and progression margin.

10:50 AM

Automated Stub Inspection System for Söderberg Technology: *Jean-Pierre Gagne*[1]; René Minville[1]; Denys Bérubé[2]; Leonardo Paulino[3]; Gilles Dufour[4]; [1]STAS; [2]Alcoa Aluminerie de Baie-Comeau; [3]Alumar; [4]Alcoa Aluminerie de Deschambault

In the Söderberg process, steel stubs – inserted directly into the anode paste of the electrolysis cell – have to be changed every 15 18 days. Their shape and length are critical to ensure good electrical distribution and avoid anode breakage. After each cycle, stubs are cleaned and manually inspected by operators to determine whether they will be sent back to production or to the repair area. Stubs with improper lengths are rejected using a Go gauge; those with improper shapes are rejected according to the operators' judgment, thus with highly variable

results. Furthermore, some eroded shapes that could cause the anode block to crack during stub extraction are difficult to spot. The Alcoa-STAS R&D team has developed an automated stub inspection system that measures and classifies stubs. The information is saved in a database used to characterize stub population, prepare schedules and forecast costs of stub repairs.

11:10 AM

Logistic Simulation of Discrete Material Flow and Processes in Aluminum Smelters: *Anton Winkelmann*[1]; Ingo Eick[1]; Christian Droste[1]; Martin Segatz[1]; [1]Hydro Aluminium

Aluminium production depends on a multitude of different operations requiring discrete transport of materials more than twice as much as metal produced. The efficient integration of additional transport and process demand due to capacity creep or brownfield expansion into the existing infrastructure is intricate. Hydro Aluminium has a long history in solving the logistic challenges using simulation tools. Limitations of the existing models concerning model set-up and control logic suggested the development of a more flexible, modular and powerful simulation tool. The targeting range of applications includes the evaluation of transport logistics of existing smelters, but also the optimization of new mega smelter designs, new potroom operating concepts and support of investment decisions. The paper outlines the relevant discrete material flows, processes and procedures and some details of the model architecture. Examples highlight the range of applications and illustrate the outcome and gain of the systematic simulation approach.

11:30 AM

Potroom Metal Treatment by Charcoal Filtration - Removing Lithium and Other Alkaline Metals from the Aluminum: *André Abbe*[1]; [1]TRIMET ALUMINIUM AG

The Hamburg smelter, which was started in 1974, is now operated by TRIMET ALUMINIUM AG since December 2006. The potlines are equipped with 180 kA side-by-side Reynolds P19 cells. The electrolyte was lithium modified to reduce the liquidus temperature and increase the bath conductivity. The lithium content in the bath of roughly 3 wt% caused a lithium contamination of the aluminum of 20 ppm. This level is harmful to special products in the casthouse and metal treatment was essential. The metal filtration was done using a charcoal filter to reduce the lithium content of the aluminum by 50%. This approach was successful but to the expense of metal loss in the order of 0.3 wt%. Therefore TRIMET started changing the electrolyte composition to eliminate lithium contamination and eliminate the filtration. This paper discusses the charcoal filtration process and reflects the challenges when switching the electrolyte from lithium to non-lithium bath.

Biological Materials Science: Biological Materials II - and - Implant Biomaterials III

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Biomaterials Committee, TMS/ASM: Mechanical Behavior of Materials Committee
Program Organizers: Ryan Roeder, University of Notre Dame; John Nychka, University of Alberta; Paul Calvert, University of Massachusetts Dartmouth; Marc Meyers, University of California

Thursday AM — Room: 3014
February 19, 2009 — Location: Moscone West Convention Center

Session Chairs: Marc Meyers, University of California; Po-Yu Chen, University of California, San Diego

8:30 AM Invited

Nanomechanics of Biological Systems — What Can We Learn from Nature about the Principles of Hierarchical Materials?: *Huajian Gao*[1]; [1]Brown University

Mechanics of hierarchical materials inspired by nature may provide useful hints for materials engineering. Some questions of interest include: what are the roles and principles of structural hierarchy? What determines the size scales in a hierarchical material system? Is it possible to design hierarchical materials with designated mechanical and other properties/behaviors? The present talk will be focused on the basic mechanics principles behind hierarchical materials. We perform detailed analyses on two idealized, self-similar models of hierarchical materials, one mimicking the mineral-protein composite structure of bone and bon-like materials, and the other mimicking gecko's attachment system, to demonstrate that structural hierarchy leads to simultaneous enhancement/optimization of multiple mechanical properties/functions such as stiffness, toughness, flaw tolerance and work of adhesion.

9:00 AM

Hierarchy Correlations in Atomistic Mechanics of Collagen Hydroxyapatite Biomimetic Composites: Devendra Dubey[1]; *Vikas Tomar*[1]; [1]University of Notre Dame

One of the motivations in developing biomimetic materials is the use of complex structural hierarchy to obtain materials with fault tolerance. Another interest is in using hierarchy to couple with additional functional properties. In this work, we present our extensive atomistic hierarchical analyses of tropocollagen (COL) and hydroxyapatite (HAP) nanocomposite interfaces. Focus is on understanding the role of hierarchy in peak interfacial strength for fracture and in determining the extent of the localization of peak fracture stress. We find that the crystalline orientation, supercell dimensions, collagen residue sequence, and volume fraction are important factors crucial to the overall hierarchical fault tolerant design. We also analyzed COL-HAP nanocomposites in three different chemical environments: vacuum, water, and calcinated water. Simulations show a clear correlation between the concentration of the surrounding environment and the predicted mechanical properties. We also found that environment could be coupled with multitude of functional properties in such bio-nanocomposites.

9:20 AM

Advanced Characterization of Biological Materials via Microstructure Correlation Functions: *Stephen Niezgoda*[1]; David Turner[1]; Haviva Goldman[1]; Ulrike Wegst[1]; Surya Kalidindi[1]; [1]Drexel University

The internal structure of biological materials has been optimized by evolution and is primarily responsible for the unmatched combination of properties seen in materials such as wood, shell and bone. For many bio-materials this internal structure is extremely complex exhibiting structural anistoropies and heterogeneities that span several length scales. The challenges posed by biomimetic design require a more complete structure description than volume fraction based metrics such as pore size distributions and more advanced homogenization relationships than simple rule-of-mixtures bounds. To this end we present a mathematically rigorous description of internal structure based on a hierarchy of higher-order statistical functions (n-point correlations). In particular we will demonstrate the utility of 2-point correlation functions in characterizing the inherent variability in a materials structure and properties, generating representational volume elements and quantification of the similarities or differences between materials and samples on a range of biological materials including cancellous bone and wood.

9:40 AM

Traumatic Brain Injury: Constitutive Modeling of the Porcine Brain under Large Deformation: *Raj Prabhu*[1]; Mark Begonia[2]; Jean-Luc Bouvard[1]; Lakiesha Williams[2]; Jun Liao[2]; Esteban Marin[1]; Doug Bammann[1]; Mark Horstemeyer[1]; [1]Center for Advanced Vehicular Systems, Mississippi State University; [2]Department of Agricultural and Biological Engineering, Mississippi State University

Brain is one of the most critical organs of the human body during life-threatening and injury sustaining accidents. According to Center for Disease Control reports, Traumatic brain injury (TBI) is a leading cause of death and life-long disability in the United States. Current finite element (FE) models lack accurate descriptions of the mechanical behavior of the brain. Without an accurate representation of the history-based constitutive models of various components, predictive capabilities of these FE models are limited. The primary goal of this research effort is to develop a history-based internal state variable constitutive model for the mechanical behavior of porcine brain. The constitutive model equations are framed in a thermodynamics setting using large deformation kinematics that accounts for history dependence and microstructure-property relations for damage. The parameters of the model have been calibrated using stress-strain responses obtained from both quasi-static and high rate tests performed on porcine brain samples.

10:00 AM Break

10:10 AM
Field-Assisted Sintering of Nanocrystalline Hydroxyapatite for Biomedical Applications: *Tien Tran*[1]; James Shackelford[1]; Joanna Groza[1]; [1]University of California

A recognized bioactive ceramic, hydroxyapatite (HA) is an excellent candidate in biomaterials selection. By reducing grain sizes to the nanocrystalline level, protein adsorption and cell adhesion are enhanced while strength, hardness, and wear resistance are improved. Unfortunately, the low phase stability, poor sinterability, and tendency towards exaggerated grain coarsening make it difficult to isolate the fracture toughness-grain size relationship from porosity effects by conventional sintering methods. The field-assisted sintering technique (FAST) is capable of heating rates up to 1000°C/min, thereby minimizing the low temperature exposure time of the powders when grain coarsening is active, but densification is minimal. Fully dense, transparent nanocrystalline HA has been consolidated by FAST in fewer than 20 minutes. While no decomposition was detected by XRD, the degree of dehydroxylation was assessed by simulated body fluid immersion tests. Fracture toughness was measured by both microindentation and single-edge v-notch bend (SEVNB) testing.

10:30 AM
Synthesis of Hydroxyapatite Nanopowders Using Induction Plasma Spray: Mangal Roy[1]; Amit Bandyopadhyay[1]; *Susmita Bose*[1]; [1]Washington State University

Calcium phosphate (CaP) materials, especially hydroxyapatite (HAp) and tricalcium phosphate (TCP), gained significant importance as bone substitutes, fillers and coating materials due to their compositional similarities with natural bone. Nanoscale CaP materials has the ability to promote intimate bone growth and improve mechanical properties of dense compacts. In our work, HAp nanopowder was synthesized using inductively coupled radio frequency solution plasma spray with HAp sol as precursor. HAp sol was axially fed into the RF plasma jet at different plasma powers between 20 and 30kW. Particle size, surface area, morphology and phase composition of the synthesized powders were characterized using TEM, XRD, FTIR, particle size analyzer and BET surface area. High purity spherical HAp nanopowders were synthesized in large scale with particle size in the range of 40-80 nm. The presentation will focus on influence of induction plasma spray parameters on HAp nanopowder synthesis and process yield.

10:50 AM
Influence of Citric Acid on the Formation of Hydroxyapatite Powders: *Chang Qing*[1]; Ru Hongqiang[1]; Yu Liang[1]; Zhang Xiantie[1]; Li Jiguang[1]; [1]Northeastern University

Citric acid (CA) is known as a strong chelating agent for metallic ions. Our purpose is to study the influence of CA on the formation mechanism and properties of hydroxyapatite (HA). The nano-HA powders were synthesized by a simple sol-gel method using Ca(NO3)2•4H2O and P2O5 as precursors, with CA as an additive. For comparison, gels without CA were also prepared. The addition of CA promoted HA formation, and the powders calcined at 320° contained the HA phase, though exhibiting low crystallinity. Under identical calcination conditions, the gel without CA showed an intense XRD peak of CaO, but that with CA showed major peaks of HA and a very weak CaO peak. Thus CA played an active role in reducing CaO content. Results also showed that the synthesized HA powders from gels with CA were finer than those without CA.

11:10 AM
Design and Fabrication of Nanocomposites for Biomedical Applications: *Iris Rivero*[1]; [1]Texas Tech University

Materials for biomedical applications, such as orthopedic implants, must be designed with several criteria in mind: 1) biocompatibility, 2) mechanical properties resembling those of bones, and 3) and efficient processing. Overall, nanocomposites can provide increased strength, improved toughness, higher thermal expansion coefficient, with reduced elastic modulus and density. For orthopedic implants it is expected that nanocomposites will improve osteoblast and osteoclast functions, and decrease fibroblast functions, in comparison with microstructured materials. This research will consider titanium and hydroxyapatite as constituents for the suggested biocompatible nanocomposites. Fabrication of the biomedical nanocomposites will be achieved by means of ball mill grinding at room temperature. Fabrication of the nanocomposites will be followed by characterization of the resultant grain size, morphology, and composition of the material. At the end, this research will identify the effect of processing parameters as milling temperature, time, and volume proportion of titanium and hydroxyapatite on resultant grain size.

Bulk Metallic Glasses VI: Structures and Mechanical Properties III

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: 3007
February 19, 2009 Location: Moscone West Convention Center

Session Chairs: Yoshihiko Yokoyama, Institute of Materials Research; Tohru Yamasaki, University of Hyogo

8:30 AM Invited
Ordered Cluster and Free Volume in a Zr-Ni Metallic Glass: X. J. Liu[1]; *G. L. Chen*[1]; X. Hui[1]; Z. P. Lu[1]; [1]University of Science and Technology Beijing

In this work, the atomic arrangement of a model metallic glass (MG) Zr2Ni was studied by extended x-ray absorption fine structure and x-ray scattering experiments combined with reverse Monte Carlo (RMC) simulation imposed an additional potential constraint. By an approach to calculate the free volume (FV) on atomic level, we have found a connection between the coordination number and FV, and then revealed that the atomic structure of Zr2Ni MG is essentially an association of ordered clusters and FV. The ordered clusters about 1.5 nm consist of a densely packed core (i.e., icosahedral-type packing) and the surrounding loosely packed clusters with large FV. The decreasing potential energy during RMC simulation proves that the associated structure is a more stable structure. This finding not only will facilitate the understanding of atomic structure of MGs, but also may provide fundamental insights into the explanation of their unique mechanical behaviors.

8:45 AM
Fracture of $(Cu_{50}Zr_{50})_{100-x-z}Al_xY_z$ Bulk Metallic Glasses: Paolo Matteis[1]; Pasquale Russo Spena[1]; Chiara Pozzi[1]; *Donato Firrao*[1]; Tanya Baser[2]; Marcello Baricco[2]; Jurgen Eckert[3]; Livio Battezzati[2]; Jayanta Das[3]; [1]Politecnico Di Torino; [2]Università di Torino; [3]IFW Dresden

The interplay between chemical composition, plastic behavior, and fracture modes of $(Cu_{50}Zr_{50})_{100-x-z}Al_xY_z$ (x=4, 5, 7 and z=0, 5) bulk metallic glasses was investigated by compression test and fracture surfaces analyses, to explore the possibilities of coupling physical, chemical and hardness properties, on one side, with adequate macroscopic compression plasticity, on the other side. Compression cylindrical test samples, having a height-to-diameter ratio equal to 2, were machined and ground from as-cast bars, and were loaded between lubricated plates, the displacement being measured by a clip-gage inserted between the plates.As a function of Al and Y content, the engineering stress-strain curves may show a plastic behavior consisting of successive sudden stress drops and linear reloading segments (evident in the absence of Y). These features, as well as the number of serrations, were statistically examined. Rupture surfaces were observed by SEM to ascertain the influence of composition on the varying fracture mechanisms.

8:55 AM Invited
Viscous Flow Behaviours of Zr-Cu-Al-(Ni) Bulk Metallic Glasses over the Entire Temperature Range: *Tohru Yamasaki*[1]; Yosuke Tanimoto[1]; Yoshihiko Yokoyama[2]; Takehiko Ishikawa[3]; Akihisa Inoue[2]; [1]University of Hyogo; [2]Tohoku University; [3]Japan Aerospace Exploration Agency

Viscous flow behaviors of $Zr_{55}Cu_{30}Al_{10}Ni_5$ and $Zr_{55-x}Cu_{35+x}Al_{10}$(x=0, 5, 10 at. %) bulk metallic glasses over the entire temperature range containing supercooled liquid region and the equilibrium liquid region has been examined. Viscosity has been measured by using a penetration viscometer under various heating rates in the supercooled liquid region and a containerless electrostatic levitation method in the equilibrium liquid region. In the supercooled liquid region, the viscosity decreased with increasing the heating rate and tended to saturate at the heating rate of 200°C/min and above. So, acceptable results were obtained at the heating

rate of 200°C/min and above. This may partly reflect a decrease in the oxygen contamination. In the equilibrium liquid region, the viscosity exhibited very low values that are about $1x10^{10}$ times lower than that of the supercooled liquid. The viscosity of these Zr-Cu-Al-(Ni) supercooled liquids and equilibrium liquids has been fitted by a Vogel-Fulcher-Tammann (VFT) relationships.

9:10 AM

Strain Distribution in Bulk Metallic Glasses Investigated by In-Situ Tensile Tests under Synchrotron Radiation: *Mihai Stoica*[1]; Jayanta Das[1]; Jozef Bednarcik[2]; Wei Hua Wang[3]; Jürgen Eckert[1]; [1]IFW Dresden; [2]HASYLAB Hamburg; [3]Institute of Physics, Chinese Academy of Sciences

We report on the evolution of the atomic-scale strain tensor of ductile $Zr_{64.13}Cu_{15.75}Ni_{10.12}Al_{10}$ bulk metallic glass under tensile loading by using x-ray synchrotron radiation. The same kind of samples was previously investigated under compressive loading and revealed yielding at 1690 MPa together with large deformability of up to 160% strain. In tension the samples fracture at a lower stress, 1500 MPa, with no sign of yielding or plastic deformation. With no macro-plasticity observed under tension, large differences in the elastic constants obtained from the strain tensor and from ultrasonic sound velocity measurements are revealed. The work presents in detail the measuring procedure as well as the calculation of the tensile tensor and pair distribution functions of $Zr_{64.13}Cu_{15.75}Ni_{10.12}Al_{10}$ at different stages of deformation. The results are discussed in comparison with other reported data obtained from x-ray diffraction measurements using synchrotron radiation.

9:20 AM Invited

Solid State Bonding of Zr Based and Cu Based BMG: *Shing-Hoa Wang*[1]; Pei-Hung Kuo[2]; Peter K. Liaw[3]; Guo-Jiang Fan[3]; Hsiao-Tsung Tsang[4]; Dongchun Qiao[3]; Feng Jiang[3]; [1]Department of Mechanical Engineering, National Taiwan Ocean University; [2]Institute of Materials Engineering, National Taiwan Ocean University; [3]Department of Materials Science and Engineering, The University of Tennessee; [4]Chung-Shan Institute of Science and Technology

Limitations and difficulties with the welding and joining of bulk metallic glasses (BMGs) are caused by cracks formed by brittle recrystallization compounds produced during welding of interfacial zones of joints. The previous research works of the welding on Bulk Metallic Glass will be reviewed. A fully amorphous phase of similar S1(Cu60Zr30Ti10)/S1(Cu60Zr30Ti10) and S3(Zr52.5Cu17.9Ni14.6Al10Ti5)/ S3(Zr52.5Cu17.9Ni14.6Al10Ti5) BMGs joints and a dual-amorphous phase of dissimilar S1(Cu60Zr30Ti10)/S3(Zr52.5Cu17.9Ni14.6Al10Ti5) BMGs joints have successfully been developed at the interface. Furthermore BMG with Sc addition (Zr55Cu30Ni5Al10)99.98Sc0.02 shows an excellent stable glass forming ability (GFA). The fusion zone of BMG (Zr55Cu30Ni5Al10)99.98Sc0.02 remains in the same amorphous state as that of the amorphous base metal when the weld is cooled with accelerated cooling.

9:35 AM

Mechanical Properties of Mg58Cu31Y6Nd5 BMG Composites with the Porous Mo Dispersion: *Hsieh Pei-Ju*[1]; Su Hsiao-Chun[1]; [1]I-Shou University

The base alloys of Mg58Cu31Y6Nd5 BMG rods are made by injection casting. Vickers indentation and compression test are performed for the mechanical properties measuring. The fracture toughness is ~8 MPa m1/2 and the fracture behavior of the compressive tests is brittle. For the mechanical properties promotion, the Mo particles are selected to be an additive in the base alloy. Then the results of the compressive tests for Mg58Cu31Y6Nd5-Mo BMG composites revealed that the plastic strain is improved with the addition of Mo particles (~5.2%). Vein-patterns are spread on the fracture surface. The fracture toughness is also improved (~25 MPa m1/2 for Mg58Cu31Y6Nd5 -20 vol% Mo). SEM observation of BMG composites reveals that the addition of Mo particle for resisting the shear bands and cracks propagation is contributive. Shear bands are stopped at the Mo particles and secondary shear bands are formed during the plastic deformation process.

9:45 AM

Chemical Composition Effect on the Mechanical Behaviour of Zr-Based BMG: *Yannick Champion*[1]; Sophie Nowak[1]; Patrick Ochin[1]; Alexander Pasko[1]; [1]Centre National De La Research Sci

Metallic glasses are known for exhibiting strong stress-strain localisation in shear bands which gives rise to absence of macroscopic ductility. The mechanisms of initiation and propagation of shear bands have been described by the monatomic free volume model proposed by Spaepen and subsequently by its extension to group of atoms developed by Argon. This can be examined experimentally through the activation volume (or more precisely "apparent activation volume" since it depends on the type of testing), which is the thermally activated volume of matter involved in the rate controlling process. Shear band initiation and then mechanical behaviour should be dependant on, and then controlled by average atomic bonding energy. Variation of the activation volume was analysed using nano-indentation with respect to the chemical composition in order to evaluate local effect of various atoms such as W, Ta, Sn on the mechanical behaviour of Zr-based BMG.

9:55 AM Break

10:05 AM

Size Effect on the Deformation and Yield Strength of Zr50Cu37Al10Pd3 Metallic Glass Micro-Pillars: *Yong Yang*[1]; [1]the Hong Kong Polytechnic University

We report our recent experimental findings, in the micro-compression tests at a constant strain rate, of the size effect on the deformation and yield strength of the Zr-based metallic glass micro-pillars. At a fixed pillar's height, the reduction of the pillar's diameter from the micron to submicron scale led to a gradual transition of the plastic deformation modes from successive to intermittent shear banding, and eventually to homogeneous deformation at the pillar's diameter of ~ 700 nm. Accompanying the deformation mode transition, an increase in the apparent initial yield strengths was also observed.

10:15 AM

Correlation of Atomic Structure with Kinetic and Elastic Properties in Zr- and Cu Based Bulk Metallic Glasses: *Xidong Hui*[1]; Guoliang Chen[1]; [1]University of Science and Technology Beijing

Ab initio molecular dynamics(AIMD) calculations were performed on the atomic configuration, kinetic properties and elastic constants of Zr-Ti-Cu-Ni-Be and Cu-Zr-Al bulk metallic glass. The local structures were characterized in terms of structure factors, pair correlation functions, coordinate numbers, bond pairs and Voronoi polyhedra. The glass transition temperature, generalized PCF and SF predicated by AIMD were compared with experimental data. Short- and medium-range orders are extracted from the atomic configurations. The diffusion coefficients and viscosities of the undercooled liquid, and the elastic constants of these two bulk metallic glasses were calculated. Based on these calculation results, the correlations of atomic structure with the elastic property, fragility and glass forming ability were discussed in detail.

10:25 AM

Size Dependence of Compressive Strength of a Zr-Based BMG: *W.F. Wu*[1]; Yi Li[1]; [1]National University of Singapore

A sample size dependence of the compressive strength has been established for a Zr-based bulk metallic glass (BMG) with a statistical method. Two competing factors, namely, free volume effect and flaw-sensitivity effect were found to affect the apparent strength of BMGs with different specimen sizes. As a result, there was a critical size with which the strength of BMG reached a maximum. In addition, a size dependence of Weibull modules was observed which is attributed to the fact that the resulted BMG samples possessed various structural configurations due to the different size dependence cooling rate. The decrease in Weibull modulus as the sample size increases indicates a deterioration of mechanical reliability for larger-sized BMG component.

10:35 AM Invited

Thermodynamic Calculation and Microstructure Evolution in Phase Separating Metallic Glass Alloys: H. J. Chang[1]; E. S. Park[2]; W. Yook[3]; J. S. Kyeong[3]; W. T. Kim[4]; *Do-hyang Kim*[3]; [1]Division of Humantronics Information Materials, Yonsei University; [2]Harvard University; [3]Yonsei University; [4]Cheongju University

In the present study, various types of microstructures resulted from phase separation in liquid state have been investigated in melt spun Gd-(Zr/Ti)-Al-(Co/Cu) alloys. The existence of miscibility gaps and spinodal decomposition curve in the liquid Gd-Ti-Al-Co/Cu systems were examined by thermodynamic calculation using CALPHAD method. Considering the thermodynamic information, we can control the microstructure depending on the processing parameters (undercooling) and alloy chemistry; i.e. i) droplet and interconnected structure in terms of morphology, and ii) amorphous+amorphous phases or amorphous+crystalline phases in terms of crystallinity. Interestingly, it was found that droplet of ß-Ti phase was present in Gd-rich amorphous matrix in the Gd30Ti25Al25Cu20 alloy, and GdCu phase was present with Ti-rich amorphous phase in a complicated interconnected network structure in

the Gd30Zr25Al25Cu20 alloy. The present result suggests that using phase separation in the liquid state, a new type of amorphous-crystalline composite structure in the form of droplet/interconnected structure can be fabricated.

10:45 AM Invited
Research Activities of Bulk Metallic Glasses at Zhejiang University: *Jianzhong Jiang*[1]; [1]Zhejiang University

In this talk, we report research activities of bulk metallic glasses (BMGs) at Zhejiang University within the last four years (2004-2008). (1)We report composition optimization, thermal and physical properties of new families of La-based bulk metallic glasses with high glass forming ability (GFA) based on a ternary La62Al14Cu24 alloy. By refining (Cu, Ag)/(Ni, Co) and La/(Cu, Ag) ratios in La-Al-(Cu,Ag)-(Ni,Co) pseudo quaternary alloy system, formation of 35 mm in diameter of LaAl(CuAg)(NiCo) BMG alloy is achieved by using Cu-mold casting; (2) We report the use of in situ high energy X-ray diffraction to detect the tensile behavior of two Zr- and La-based BMGs. Based on the diffraction data, the tensile elastic modulus and Poisson's ratio can be accurately evaluated; (3) Atomic structures of bulk glass-forming Cu64.5Zr35.5 and the eutectic composition Cu61.8Zr38.2 metallic glasses (MGs) have been studied by a combination of state-of-the-art experimental techniques and computational methods.

11:00 AM
Characterization of Amorphous and Crystalline ZrCuAgAl Thin Films Deposited by Magnetron Sputtering: *Chia-Cheng Tsai*[1]; J. H. Huang[1]; G. P. Yu[1]; ChihPin Chuang[2]; Peter K Liaw[2]; [1]National Tsing-Hua University; [2]University of Tennessee, Department of Materials Science and Engineering

Amorphous and crystalline ZrCuAgAl films were deposited on p-type (100) Si and 304 stainless steel substrates by unbalanced magnetron sputtering (UBMS). The influence of structures on the mechanical, electrical, and corrosion properties of the thin films were studied. Results showed that the ZrCuAgAl thin film deposited at room temperature was in an amorphous form, while that deposited at 400°C possessed a good crystalline structure with major phases consisting of Cu10Zr7 and CuZr2. The electrical resistivity of the films was about 160 μΩ-cm. The crystalline thin films had higher hardness and elastic constants compared with the amorphous counterparts. The residual stresses for the films deposited on the Si exhibited large differences for the crystalline and amorphous forms. The stress of the crystalline film was more than 8 times higher than that for the amorphous one. On the other hand, the amorphous thin films had better corrosion resistance than the crystalline films.

Cast Shop for Aluminum Production: Casting Technology

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee
Program Organizers: Pierre Le Brun, Alcan CRV; Hussain Alali, Aluminium Bahrain

Thursday AM — Room: 2005
February 19, 2009 — Location: Moscone West Convention Center

Session Chair: Robert Wagstaff, Novelis

8:30 AM Introductory Comments

8:35 AM Keynote
Remelt Ingot Production Technology: *John Grandfield*[1]; [1]Grandfield Technology Pty Ltd

The technology related to the production of remelt ingots (small ingots, sows and T-Bar) is reviewed. Open mould conveyors, benching, sow casters, and VDC and HDC casting of T-Bar are described and compared. Process economics, capacity and product quality issues are listed. Trends in casting machine technology such as longer open mould conveyor lines are highlighted. Safety issues related to the operation of open mould conveyor casting machines for production of remelt alloy ingots are discussed. The potential hazards are listed. One of the main risks is the potential for molten metal ejections during mould filling. The advantages and disadvantages of the various machine configurations and options such as dry filling with the mould out of water and wet filling with the mould in water are discussed. The effect of mould design on machine productivity, mould cracking and mould life is also examined.

9:05 AM
Nanotechnology Breakthrough Optimises Casting Process: *Volker Hofmann*[1]; [1]ItN Nanovation AG

With Nanotechnology it is possible to create a ceramic coat by using process given temperatures. A suspension containing nanoscalic particles, sprayed thinly on the substrate, sinters to a robust and heat resistant ceramic by 300-400°C (600 – 750°F). It is not required to sinter the coat in a pre heating process. Sintering while melt contact leads to the expected result. So the robustness of a ceramic applies to moulds launders and dies. This can be achieved by simple maintenance operation on the shop floor. High service time provided by a very thin coat avoids coat build-up and leads to process stability.

9:25 AM
A Simplified Method to Characterize Mold Cooling Heat Transfer and an Experimental Study of Impacts of Water Temperature on Ingot Casting: *Sebastien Bolduc*[1]; Ho Yu[2]; Laszlo Kiss[1]; [1]University of Quebec; [2]Alcoa Technical Center

The heat transfer characteristics of mold cooling water are of great interest in ingot casting. A question often arises, when there is a bleed-out or cracking problem, is how much cooling water should one increase or decrease to correct the problem. To characterize the cooling water heat transfer of a mold is time consuming. It usually needs numerous heat transfer measurements in an experimental setup under different cooling water conditions, e.g. flow rate, water temperature and chemistry, etc. This paper presents a unique method to characterize the cooling water heat transfer of a mold. The method determines the Leidenfrost temperatures, reducing greatly the amount of effort needed to generate the mold heat transfer correlations. The correlations can then be used as guidelines to adjust cooling water flow rate or as boundary conditions for an ingot mathematical model. As an example, the effects of water temperature on ingot casting are presented.

9:45 AM
Advances in Cooling Water Deposit Control for Direct Chill Ingot Casting: *Yves Lefebvre*[1]; Caroline Sui[1]; Wilson Whitekettle[1]; [1]GE Water and Process Technologies

In aluminium DC casting, maintaining the integrity of heat transfer at the mould-water interface is of utmost importance from a productivity and surface quality standpoint. Heat extraction is critical and the focus of cooling water treatment is to keep this high temperature surface free of deposits. This paper discusses two new-generation products that have been recently developed to control two very troublesome types of deposits as far as resistance to heat transfer: biofilms and mineral scales. Furthermore, biofilms are a health concern as they provide favourable conditions for growth of the Legionella bacteria. The first product is a non-foaming biofilm remover, the second one is a polymer to control phosphate, iron and aluminium deposits. Laboratory data using cooling tower simulation equipment will be presented along with preliminary field applications.

10:05 AM Break

10:25 AM
Heat Transfer During Rod Casting: *Laurent Cottignies*[1]; Vincent Duhoux[1]; Soizic Blais[1]; Celio Duran[1]; [1]RioTinto Alcan

This work contains the description of a heat transfer model which was specially developed for the aluminium rod casting process. A two dimensional finite element formulation was used to describe the temperature field within the solidifying bar, the copper mould and the steel belt. The focus of this work was on heat transfer coefficients at interfaces. Heat fluxes at aluminium-mould and mould-water interfaces were estimated by inverse heat transfer analysis, using dedicated temperature measurements. Significant differences were registered between various locations along the aluminium-mould interface. Thermo mechanical calculations and experimental characterizations of the casting surfaces were used to understand in more detail the factors controlling heat transfer.

10:45 AM
Prevention of Starting Cracks in Al-Billets: Feasible Methods for Float and Spout DC-Casting: *Marcel Rosefort*[1]; Thomas Koehler[1]; Hubert Koch[1]; [1]Trimet Aluminium AG

Hot crack formation especially starting crack formation in butts of DC cast extrusion billets often causes rejections, in particular while casting high-alloyed aluminum. The prevention of such starting cracks can reduce the rejection rate

noticeable. Crack formation is well investigated in theory and many techniques for crack prevention are used in practice. Nevertheless starting cracks are a problem in DC casting. This paper presents an investigation on methods to prevent starting cracks in Al-billets production using float and spout DC-casting. Starting with the results of former investigations and practical experience these methods are tested for there suitability for crack prevention. The main focus was to apply all technologies to the float and spout DC-casting. The paper presents the research methods, the results of crack prevention and the real implementation in practice.

11:05 AM

Improving the Surface of AA6111 Sheet Material, Cast at High Speeds, through the Use of Macroscopically Textured Substrates: *Donghui Li*[1]; Luis Calzado[1]; Mihaiela Isac[1]; Roderick Guthrie[1]; [1]McGill Metals Processing Centre

The surface topography and coating materials of water cooled belts greatly affect interfacial heat flows, strip surface quality, and as-cast microstructures, for thin strips cast on high speed horizontal single belt casting machines (HSBC). The purpose of this paper was to investigate the surface quality of the strip by casting Aluminum AA6111 alloy on an HSBC simulator using a copper mould with different macroscopic surface textures and coatings. The transient interfacial heat flows were measured by thermocouples embedded in the copper mould. Ab-initio heat flows between the melt and the mould were predicted by mathematical modeling and favorably compared with experimental heat fluxes. It was found that the mould surface texture and coatings could be optimized to mitigate casting defects caused by air pockets entrained at the interface between the melt and rapidly moving mould. Attendant improvements in as-cast microstructures were obtained.

11:25 AM

Reinventing Twin Roll Casting for the 21st Century: *Enrico Romano*[1]; Chris Romanowski[1]; [1]Fata Hunter

The invention of twin roll casting in 1956 profoundly influenced the Western aluminum industry. The original twin roll casters were low cost machines that economically converted a variety of common alloys into sheet and foil products for the rapidly growing post-war consumer market. To meet market demand for an ever increasing range of alloys and widths, twin roll casters then became progressively bigger, more complex and costly.In recent years the economic growth in developing markets such as India has produced a surge in demand for low cost aluminum products that mirrors the Western post-war economic boom. To meet the requirements of these markets, FATA Hunter has developed a low cost casting machine that combines the low capital and operating costs of the original 1950s casters, with the latest in twin roll casting technology. The design features of this new caster are described and contrasted with a typical large machine.

11:45 AM Concluding Comments

Characterization of Minerals, Metals and Materials: Characterization of Microstructure of Properties of Materials V

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division, TMS: Materials Characterization Committee, TMS/ASM: Composite Materials Committee

Program Organizers: Toru Okabe, University of Tokyo; Ann Hagni, Geoscience Consultant; Sergio Monteiro, State University of the Northern Rio de Janeiro - UENF

Thursday AM
February 19, 2009

Room: 3009
Location: Moscone West Convention Center

Session Chairs: Lawrence Murr, University of Texas; Sergio Monteiro, State University of the Northern Rio de Janeiro - UENF

8:30 AM

Data Driven Reduced Order Models for the Representation of Polycrystalline Microstructures: *Nicholas Zabaras*[1]; Baskar Ganapathysubramanian[2]; [1]Cornell University; [2]Iowa State University

The stochastic analysis of a system requires the availability of appropriate input models of the uncertain variables. Constructing reliable input stochastic models from limited data/information is therefore an important prerequisite for the realistic analysis of complex systems. This is particularly true during physical process modeling in polycrystalline microstructures where the amount of microstructural data is limited or only available in coarse-grained form. We investigate various dimensionality reduction strategies to construct compact, data-driven reduced order models of polycrystalline microstructures. In particular, we compare and analyze features of linear model reduction strategies based on Principal Component Analysis as well as non-linear model reduction strategies based on ideas from manifold learning.

8:45 AM

Development of a Portable Load-Depth Sensing Indentation System for Online Material Characterization: Chuanyu Feng[1]; Jared Tannenbaum[1]; *Bruce Kang*[1]; Mary Anne Alvin[2]; [1]West Virginia University; [2]National Energy Technology Laboratory

Indentation technique has a unique position for online material characterization. However, due to the complexity of the indentation depth and/or contact area measurement, current portable indentation instruments are solely developed for the purpose of hardness measurement. Powerful load-depth sensing indentation can be performed only in the lab. Due to this, a load-based indentation technique suitable for field applications has been developed, which does not need any direct measurement of the contact area or depth of indentation. The new technique bears the same theoretical background as traditional load-depth sensing indentation. Additionally, by applying a multiple-partial unloading procedure, the indentation system developed using this technique involves much less cost compared to current commercial products. To demonstrate the feasibility, a portable indentation system suitable for online material characterization has been developed. Excellent measurement results have also been obtained.

9:00 AM

Safety Characterization of Electrical Systems in Diesel Electric Locomotive: *Jeongguk Kim*[1]; Chang-Young Lee[1]; Seung-Koo Baek[1]; Sung Cheol Yoon[1]; [1]Korea Railroad Research Inst

In diesel electric locomotives, which were used for over 25 years, the characterization of electrical system was conducted for deterioration and safety evaluation through insulation resistance measurement, degradation testing, and infrared thermography method. Especially an infrared camera and thermocouples were employed for the evaluation. The thermocouples were attached on high-voltage cables connected to traction motors, for in-situ measurement of abnormal heating during test running. After test running, the thermographic images were obtained for the inspection of high-voltage cables using the infrared camera. The thermographic results were quantitatively analyzed, and compared with temperature changes during running. In this investigation, various analysis techniques for the safety characterization of diesel electric locomotives have been introduced, and the analysis results have been used to provide the deterioration or wear information in current locomotive systems.

9:15 AM

Characterization of Hot Spots Generation in Railway Brake Disc: *Jeongguk Kim*[1]; Byung Choon Goo[1]; Sung Cheol Yoon[1]; Sung-Tae Kwon[1]; [1]Korea Railroad Research Inst

The generation of hot spots on railway brake disc was investigated using the infrared thermography method. In brake system, the hot spots on the surface of brake disc have been considered as thermal distortions with high thermal gradient, and the control of hot spots has been an important issue for the lifetime extension of brake disc. In this investigation, a brake disc with gray cast iron, which is currently used in Korea, was employed. A high-speed infrared (IR) camera was used to measure the surface temperature of brake disc as well as for in-situ monitoring of hot spot evolution during braking operation. From the thermographic images, the observed hot spots and thermal damage of railway brake disc during braking operation were qualitatively analyzed. Moreover, the previous experimental and theoretical studies on hot spots phenomenon were reviewed, and the current experimental results were introduced and compared with theoretical prediction.

9:30 AM

Mechanical Properties and Fracture Toughness Evaluation of Structural Steel with the Emerging Ball Indentation Technique and Its Numerical Validation: *Sabita Ghosh*[1]; Mita Tarafder[1]; S Sivaprasad[1]; Soumitra Tarafder[1]; [1]National Metallurgical Laboratory

Among various small specimen and minimally invasive techniques to determine mechanical properties of materials, the ball indentation technique (BIT) has proved to be advantageous. BIT is used when a tensile test cannot be performed: on welded joints or components under service. The present work highlights the applicability of BIT to evaluate flow behaviour of engineering structural steels. Mechanical properties like ultimate tensile strength, yield stress, strain hardening coefficient evaluated for steels with varying heat treatment and mechanical working conditions. To determine fracture toughness from the flow curve, non linear damage models have been utilized. Attempt has been made to model the crack initiation, propagation and finally the fracture behaviour at different aging conditions using the results generated by the BIT. These results are compared with the same obtained by conventional tests. Validation of the BI test results has been carried out by Finite Element Modelling using ABAQUS software package.

9:45 AM

Characterization of Cantera Stone from Hidalgo State, México: Viability Study for Recycling and Reusing of Wastes: *Eleazar Salinas*[1]; Juan Hernández[1]; Francisco Patiño[1]; Eduardo Cerecedo[1]; Marius Ramírez[1]; Martín Reyes[1]; Miguel Pérez[1]; [1]Universidad Autónoma del Estado de Hidalgo

This work is related with a whole characterization of cantera stone, to establish its characteristics that can give it an additional value for its reuse and reutilization of dust, slurries and small pieces of stone which can be treated as wastes. The obtained results reflects that the residues studied can be used as substitutes of feldspars in the production of pieces of ceramic, and also in the elaboration of paints for the same pieces according to the mixes that can be made with the variation of Na2O, CaO and K2O. According to the humidity proofs and specific gravity done, this material can be proposed as a soil improver into hydroponics systems, leading so an important alternative for food production in zones leaking of water. In the same way, it was found the possibility of use this material as a seal 3A in processes of asphalting of roads, highways and streets.

10:00 AM Break

10:20 AM

Izod Impact Energy of Polyester Matrix Composites Reinforced with Aligned Curaua Fibers: *Sergio Monteiro*[1]; Ailton Ferreira[1]; Felipe Lopes[1]; [1]State University of the Northern Rio de Janeiro - UENF

Polymer matrix composites have been applied in components such as helmets and shieldings for which toughness is a major requirement. Natural fiber present interfacial characteristics with polymeric matrices that favor a high impact energy absorption by the composite structure. The objective of this work was then to assess the Izod impact resistance of polymeric composites reinforced with different amounts, up to 30% in volume, of a promising high strength natural fiber from the Amazon region known as curaua. The results showed a remarkable increase in the notch toughness with the amount of incorporated curaua fibers. This can be attributed to a preferential debonding of the fiber/matrix interface, which contributes to an elevated absorbed energy.

10:35 AM

Statistical Analysis to Characterize the Uniformity of Mechanical Properties of Buriti Fibers: *Sergio Monteiro*[1]; Felipe Lopes[1]; Ludy Motta[1]; Leandro Marques[1]; [1]State University of the Northern Rio de Janeiro - UENF

Lignocellulosic fibers obtained from plants like cotton, flax, hemp, sisal, jute and many others are natural materials used, since long time, in basic items such as textile, baskets, roofing and carpets. These traditional natural fibers as well as some new ones are nowadays replacing synthetic fibers as composite reinforcement owing to environmental advantages. The heterogeneous characteristic of lignocellulosic fibers is, however, a limitation for application in composites. The buriti fiber, extracted from a tropical plant tree, is recently being investigated as a possible reinforcement for polymeric matrix composites but no complete information exists regarding its mechanical behavior. The objective of this work was then to carry out a statistical analysis on the mechanical properties' uniformity of buriti fibers. By precise dimensional measurements in association with tensile tests, it was found that the mechanical properties depend on the range of the fibers' dimension.

10:50 AM

Coating Characterization in CrN Deposited by Magnetron Sputtering Method on AISI 316 Steel: *Isaías Hilerio*[1]; [1]UAM AZCAPOTZALCO

Chromium nitride (CrN) thin films were deposited on steel AISI 316 substrates by radio frequency (rf) magnetron sputtering method using sputtering of a Cr target in nitrogen ambient. CrN films were produced by varying the deposition temperature, nitrogen partial pressure and rf power density. The films coated were characterized by X ray diffraction method, quantitative energy dispersive and scanning electron microscopy. These techniques were employed to characterize their phases, chemical composition and microstructure. Additionally, micro hardness was evaluated. The results show that the mechanical properties can be varied by changing the deposition conditions.

11:05 AM

Effect of Molybdenum on the Microstructure and Thermal Expansion of Ductile Iron: *Francisco Patiño*[1]; Juan Hernández Ávila[1]; Eleazar Salinas Rodríguez[1]; Francisco Patiño Cardona[1]; Isauro Rivera Landero[1]; [1]Centro de Investigaciones en Materiales y Metalurgia, Universidad Autónoma del Estado de Hidalgo

This work studies the Molybdenum effect on the microstructure and mechanical properties of an as-cast ductile iron. For this study five ductile irons with different amounts of Molybdenum each were made in an induction furnace. In this material, nodule count and nodularity are affected by the Molybdenum additions. The iron´s matrix, nodules and the phase were analyzed using scanning electron microscopy detecting Molybdenum only in the matrix. Mechanical properties, such as hardness, microhardness, tensile strength and yield strength, show increments as the Molybdenum amount is increased. In the same way, ferrite and pearlite phases display a variation in their percentage as the contents of the alloy element increase. This element has a marked influence on the pearlite interlaminar spacing. From the obtained results we conclude that Molybdenum in these quantities dissolves in solid ferrite solution during the solidification process, improving the material´s mechanical properties.

11:20 AM

Removal Fe (III) from Dilute Solutions Containing Zn (II) by Ion Flotation Techniques: Martin Reyes Perez[1]; Francisco Patiño Cardona[1]; Miguel Perez Labra[1]; Francisco Tavera Miranda[2]; Ramiro Escudero Garcia[2]; Eduardo Cerecedo Saenz[1]; *Eleazar Salinas Rodriguez*[1]; [1]UAEH; [2]UMSNH

Iron concentration by ion flotation techniques, from sulfate solutions in presence of zinc was studied, in a laboratory flotation column by continuous mode; using a synthesized sand shell plate spargered, an anionic collector, promoters, and surfactant propilenglicol 400. Effects of experimental parameters, such as the concentration of reagent, potassium amyl xanthate, dithiophosphate, superficial gas velocity, and superficial liquid velocity, were studied in terms of the recovery and enrichment of Fe (III). The results founded, shown that the iron elimination from solution in the presence and absence of zinc (II) are 59 % and 72 % respectively. The flotation efficiencies decrease with an increase of the concentration of xanthate, and air flow rate. A best recovery was achieved, at Jg 0.1 cm/s, Jl 0.72 cm/s and a mixture of xanthate and dithiophosphate as promoter. Also was demonstrated that is possible selectively separate and concentrate iron (III) from solution containing zinc.

Computational Thermodynamics and Kinetics: Grain Growth and Recrystallization

Sponsored by: The Minerals, Metals and Materials Society, ASM International, TMS Electronic, Magnetic, and Photonic Materials Division, TMS Materials Processing and Manufacturing Division, ASM Materials Science Critical Technology Sector, TMS: Chemistry and Physics of Materials Committee, TMS/ASM: Computational Materials Science and Engineering Committee
Program Organizers: Long Qing Chen, Pennsylvania State University; Yunzhi Wang, Ohio State University; Pascal Bellon, University of Illinois at Urbana-Champaign; Yongmei Jin, Texas A&M

Thursday AM Room: 3002
February 19, 2009 Location: Moscone West Convention Center

Session Chair: Yu Wang, Virginia Tech

8:30 AM Introductory Comments

8:35 AM Invited
Quantifying the Solute-Drag Effect in Al-Mg Alloys: *Moneesh Upmanyu*[1]; Branden Kappes[1]; Anthony Rollett[2]; Seth Wilson[2]; C Roberts[2]; [1]Colorado School of Mines; [2]Carnegie Mellon University

Quantifying the effect of solutes on grain boundary kinetics is a multiscale challenge because the characteristic length scale for boundary-solute interaction is a few nanometers, as opposed to the micron scale for most grain growth problems. We present the results of combined approach that uses Monte-Carlo for quantifying solute interactions at the atomistic scale and phase field/level set for modeling grain growth at the mesoscale. The interaction energies between Al grain-boundaries and individual Mg solute atoms are reported for various high angle, tilt grain boundaries. Our results reveal large variations in the form of these interactions, in stark contrast to the typical triangular profiles assumed in most previous theoretical frameworks. Using these interaction energies as inputs in the meso-scale simulations allows us to quantify solute drag effect in the low velocity, loaded regime. The results are compared with existing experimental data on Mg concentration dependence of Al grain boundary mobilities.

8:55 AM
The Topological Evolution of Anisotropic Three-Dimensional Grain Growth: *Ian McKenna*[1]; Mogadala Gururajan[1]; Peter Voorhees[1]; [1]Northwestern University

Phase field simulations are a well accepted method for modeling the evolution of various microstructures, of particular interest is polycystalline grain growth. Many of these systems exhibit anisotropic behavior during grain growth. Therefore, it is imperative that this behavior is included in phase field models in order to accurately describe the evolution. The model employed incorporates all five macroscopic degrees of freedom, grain boundary plane and grain misorientation, dependence of the grain boundary energy. To overcome the large resource requirements for calculating the evolution of three-dimensional polycrystals with thousands of grains a finite-difference sparse-matrix algorithm was developed. The calculations illustrate the important effects that anisotropy can have on three-dimension grain growth. We compare the topological evolution of grains in both isotropic and anisotropic systems.

9:15 AM
Kinetics of Copper Precipitation in Iron: Thermal Ageing and Irradiation Effects: *Frederic Soisson*[1]; [1]CEA Saclay

The kinetics of copper precipitation in iron is modeled by ab initio calculations, Monte Carlo simulations and cluster dynamics methods. Ab initio calculations are used to compute the point defect jump frequencies of vacancies and self-interstitial atoms with dumbbell configurations. These jump frequencies are used to parameterize atomistic Monte Carlo simulations which take into account the dependence of the jump frequencies on the local atomic configuration. The simulations of copper precipitation during thermal ageing are compared with experimental studies. They reveal that copper diffusion occurs not only by migration of isolated copper atoms, but also by small copper clusters. Cluster dynamics are used to study the effect of this mechanism on the long term precipitation behavior. Under irradiation, we focus on the coupling between point defects and copper fluxes, which lead to radiation induced segregation of copper at point defects sinks. We study its consequences for the precipitation kinetics.

9:35 AM
Kinetics of Formation and Thermal and Mechanical Properties of Char Obtained by Ultra-High Temperature Pyrolysis of Polyethylene via Molecular Dynamics Simulations: *Maxim Makeev*[1]; Deepak Srivastava[1]; [1]NASA Ames Research Center

We present a molecular-dynamics simulation study of ultra-high temperature pyrolysis of polyethylene, leading to char formation via hydrogen removal and collapse of carbon network. The kinetics aspect of the study includes computations of rates of hydrogen removal and temporal evolution of carbon network via Voronoi tessellation analysis. The kinetics of dehydrogenation is quantified in terms of kinetic rate behavior as a function of pyrolysis temperature. The resultant char samples are investigated for thermal andmechanical behavior and their relation to microstructure. The thermal conductivity of char samples is studied between 10K and 500K for microstructures with different coordination numbers and ring statistics. The behavior of thermal conductivity as a function of char microstructure is explained via vibrational spectral analysis of char samples. Finally, the mechanical properties of char are studied within the framework of random network paradigm and the simulation results are compared with reported data on amorphous carbon.

9:55 AM
Numerical Investigation of Deformation-Induced Dynamic Transformation in Fe-C Alloy Using a Q-State Potts Monte Carlo Model: *Dianzhong Li*[1]; Namin Xiao[1]; [1]Institute of Metal Research

The deformation induced dynamic transformation (DIDT) of a Fe-C alloy above Ae3 temperature is simulated using a Q-state Potts Monte Carlo (MC) model. The austenite-to-ferrite transformation, dynamic recrystallization (DRX) of austenite and ferrite and the ferrite-to-austenite reverse transformation can be simulated simultaneously in one MC model by building suitable MC transition rules. Meanwhile, an affine transformation model based on vector operation is also coupled with the MC model for the first time for tracking the changes in grain shape during dynamic transformation. The influence of deformation parameters, including temperature and strain rate, on the microstructure evolution and the stress-strain curves are discussed. The simulation results show that the competition between the DRX of austenite and austenite-to-ferrite transformation causes the different microstructures and changes the shape of the stress-strain curves for the different deformation parameters.

10:15 AM Break

10:30 AM
CFD Modelling of Gas Injections in Top Submerged Lance Smelting: Nazmul Huda[1]; Jamal Naser[1]; Geoffrey Brooks[1]; *Markus Reuter*[2]; Robert Matusewicz[2]; [1]Swinburne University of Technology; [2]Ausmelt Limited

A Computational Fluid Dynamic modelling of gas injections in a top submerged lance smelting unit was developed and the effect of lance submergence was investigated. The CFD software used for this purpose was FIRE 8.52. The simulation result was validated against the experimental data by comparing the velocity fields and generation of turbulence in the bath. Water was used as the modelling fluid and air was used as the injected gas to have an understanding of the mixing process and the effect of lance submergence. The simulation results showed that deeply submerged lance provide better mixing of the bath.

10:50 AM
Computational Tools for the Design of Weldable and Creep Resistant Superalloys: *Franck Tancret*[1]; [1]Polytech Nantes

One drawback of many nickel-base superalloys is their poor weldability. In particular, cracking can occur in the mushy zone during solidification, in the so-called Brittle Temperature Range (BTR). Another type of cracking is due to the formation of intergranular liquid films, by the liquation of low melting point phases like carbides and/or intermetallics. In this work, CALPHAD-type computing tools (Thermo-Calc, Dictra) are used to predict the occurrence of these types of cracking, and to design Ni base alloys by minimizing both the BTR and the risk of γ' liquation cracking, while keeping a good phase stability and good mechanical properties in the expected service temperature range. Among others, the creep rupture resistance is estimated through the multivariate regression of existing data, using artificial neural networks or Gaussian processes. Predictions are first compared to data in the case of existing alloys, and then used to propose new weldable and creep-resistant superalloys.

11:10 AM

A Mechanism of Non-Equilibrium Grain Boundary Segregation for Intermediate Temperature Brittleness in Metals: *Tingdong Xu*[1]; Kai Wang[1]; [1]Central Iron and Steel Research Institute

The graphical representation of non-equilibrium grain segregation of impurity offers a clear solution to an outstanding fundamental scientific mystery, intermediate temperature brittleness in metals, a problem which leading researchers in the field have struggled to explain for the past 100 years. For the elevated temperature tension tests of metallic materials a test temperature must exist at which a concentration peak of non-equilibrium grain boundary segregation of impurity and a relevant ductility minimum occur. The test temperature has a critical time of non-equilibrium grain boundary segregation of impurity to be equal or close to the test isothermal time at this tension test temperature. A number of diverse experimental results from a number of different labs can be rationalized on the new mechanism of intermediate temperature brittleness suggested in present paper. Main References: [1] Xu Tingdong, Cheng Buyaun, Prog. Mater. Sci., 2004; 49(2): 109-208.

11:30 AM

A Simulation of Recrystallization on a Magnesium Alloy Using Phase Field Method for Real Time and Size in Industry Scale: *Mingtao Wang*[1]; B.Y. Zong[1]; Yan Wu[1]; Xiangang Zhang[1]; [1]Northeastern University

A model has been established to simulate the realistic spatio-temporal microstructure evolution in recrystallization of a magnesium alloy using the phase field approach. Rules have been proposed to decide the reasonable value of all the parameters in the model with physical background discussion. The thermodynamic software THERMOCALC is applied to determine the local chemical free energy of the alloy and strain energy is added to the free energy density of the grains before recrytallization. A concept of boundary range is suggested to decide the gradient parameters in addition offitting to the experimental boundary energy value. The parameter values can be regarded as a database for other similar simulations and the model is easy to adapt to other alloy systems. The simulated results show a good agreement with reported experimental measurement of the alloy at the temperatures from 300° to 400° for up to 100 minutes.

Electrode Technology for Aluminum Production: Electrode Technology - Cathodes and Inert Anodes

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee

Program Organizers: Barry Sadler, Net Carbon Consulting Pty Ltd; John Johnson, RUSAL Engineering and Technological Center LLC

Thursday AM — Room: 2003
February 19, 2009 — Location: Moscone West Convention Center

Session Chair: To Be Announced

8:30 AM Introductory Comments

8:35 AM

Formation and Dissolution of Aluminium Carbide in Cathode Blocks: *Kristin Vasshaug*[1]; Trygve Foosnæs[2]; Geir Haarberg[2]; Arne Ratvik[3]; Egil Skybakmoen[3]; [1]Hydro Aluminium; [2]Norwegian Universisty of Science and Technology; [3]SINTEF Materials and Chemistry

Today, failure of aluminium reduction cells due to wear of carbon cathode blocks is one of the main factors limiting the lifetime of the cell. Formation and dissolution of aluminium carbide plays an important role in the wear process, but the mechanisms are poorly understood. Electrolysis tests were performed, and the cathode samples were analyzed by SEM and optical microscopy to study the formation of Al_4C_3 at the surface and/or in the pores of the sample. Samples from industrial cells were also included in the study. The results showed that in areas exposed to bath, dissolution of Al_4C_3 was faster than formation, as no Al_4C_3 could be seen on the surface. On surfaces covered by sintered alumina or aluminium, a thin non-coherent layer of Al_4C_3 was observed, as well as in pores close to the cathode surface. Transport mechanisms of aluminium carbide related to the wear process will be discussed.

9:00 AM

Resistivity Change of Cathode Graphite during and after Electrolysis in Alumina Molten Salt: Noboru Akuzawa[1]; Morio Chiwata[2]; Manabu Hagiwara[2]; Yoshinori Sato[1]; Hiroshi Imagawa[1]; [1]SEC Corp; [2]Tokyo National College of Technology

Change of electrical resistivity of cathode graphite during and after electrolysis in alumina molten salt was determined at different temperatures between 870 and 980°C. Resistivity of cathode graphite decreased remarkably in the initial stage of electrolysis and then became almost constant for further electrolysis. On the other hand, resistivity increased with time by interrupting electrolysis. Just after the interruption, resistivity increased rapidly with time, followed by a characteristic plateau, and again increased towards a final steady value. Repeating of this cycle resulted in remarkable enlargement of resistivity. It should be noted that a large increasing ratio of resistivity of cathode graphite before and after electrolysis was observed at relatively low temperature such as 870°C. This observation suggested intercalated sodium is stabilized at lower temperature and the amount of sodium uptake increased during electrolysis. Correspondingly, the electrolysis at lower temperature provides an effective way for evaluation on degradation of cathode graphite.

9:25 AM

Study of Aluminum Carbide Formation in Hall-Heroult Electrolytic Cells: Abdelhalim Zoukel[1]; Patrice Chartrand[2]; *Gervais Soucy*[1]; [1]Universite de Sherbrooke; [2]Ecole Polytechnique de Montreal

The trend in the aluminum reduction industry today is that of operating cells, using graphitized carbon cathode blocks; increased current density and bath chemistry with an AlF3 excess. The resulting problem is that of accelerated wear of the graphitized cathode blocks, which is thought to be caused by the formation and subsequent dissolution of the aluminum carbide at the cathode surface. This is now recognized as one of the factors limiting the cell lifetime. We will discuss a literature review. A special laboratory test method has been also developed to elucidate the mechanism of the aluminum carbide formation. The following operational parameters are varied: current density, electrolysis with or without aluminum thin film being added during start-up and time of electrolysis. The aluminum carbide formation has been studied, using X-ray photoelectron spectroscopy, X-ray diffraction and scanning electron microscopy. The analysis of the preliminary results will be presented in this paper.

9:50 AM

The Effect of Potassium Cryolite on Costruction Materials under Electrolysis Condition: Yurii Zaikov[1]; Alexander Kataev[1]; Alexander Chuikin[1]; Nikolai Shurov[1]; *Alexander Redkin*[1]; Anton V. Frolov[2]; Alexander O. Gusev[2]; [1]Institute of High Temperature Electrochemistry; [2]Engineering-Technological Center, RUS-Engineering LLC, Rusal

Laboratory study of interaction SiC-Si3N4 with low melting electrolyte based on potassium cryolite at temperature 800°C are presented. The investigation has been carried out by two techniques: 1) thermal gravimetric - continuous weighing of the sample in molten salt; 2) 100-hours electrolysis test. The values of the corrosion rate were obtained and the interaction mechanism of the material with electrolyte was proposed. Recommendations for applicability of the SiC-Si3N4 composite in potassium containing electrolyte as lining bricks in the aluminum electrolysis cell were made.

10:15 AM Break

10:25 AM

Mechanically Alloyed Cu-Ni-Fe Based Materials as Inert Anode for Aluminium Production: *Badr Assouli*[1]; Martial Pedron[1]; Sebastien Helle[1]; Daniel Guay[1]; Lionel Roue[1]; Ambre Carrere[1]; [1]Institut National de la Recherche Scientifique

High-energy ball milling has been successfully applied to the synthesis of various materials with improved chemical, physical and mechanical properties for many applications including high-temperature corrosion resistance materials. It consists of inducing at room temperature a solid state reaction between the components of a powder mixture by repeated cold welding and fractures caused by ball-to-powder collisions. In the present study, it is demonstrated that nanostructured and monophased fcc CuxNi(85-x)Fe15 materials (with x varying from 0 to 55 wt.%) can be prepared by mechanical alloying. The study of their oxidation behaviour in air at 750°C indicates that the composition, the thickness and the growth kinetics of the oxide layer vary with the Cu content in the alloy. Aluminium electrolysis tests conducted at 700°C in 45 wt.% KF + 50 wt.% AlF3

+ 5 wt.% Al2O3 electrolyte show that the electrode stability and aluminium purity are strongly dependent on the alloy composition.

10:50 AM

Effects of Pitches Modification on Properties of TiB_2-C Composite Cathodes: *Lü Xiaojun*[1]; Xu jian[1]; Lai Yanqing[1]; Li Jie[1]; Fang Zhao[1]; Shi Yan[1]; Liu Yexiang[1]; [1]School of Metallurgical Science and Engineering, Central South University

Pitches were modified by the heat-treated method, and the properties of pitches modified at different treatment temperatures were studied. Furthermore, the effects that modified pitches used as binder on properties of TiB_2-C composite cathodes were investigated. The results showed that the coke yield and the viscosity of modified pitches increased as the treatment temperature increased. When the treatment temperature increased from 220°C to 420°C, the viscosity increased from 506 mPa•s to 27500 mPa•s and the coke yield increased from 47.21% to 69.64%. As the treatment temperature increased, the variation of cathode bulk density ($\Delta\eta_\rho$=ρBaked–ρGreen/ ρGreen)) increased and the electrolysis expansion first decreased then increased. When pitches modified at 340°C, the electrolysis expansion reached the minimum and decreased by 14.01% compared to cathodes of primitive pitches. However, when pitches modified at 420°C, it increased by 3.82%.

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

Sponsored by: 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: Energy Committee, TMS: Nanomaterials Committee, TMS: Superconducting and Magnetic Materials Committee, TMS: Thin Films and Interfaces Committee
Program Organizers: Long Qing Chen, Pennsylvania State University; Mark Palmer, Kettering University; Sung Kang, IBM Corp

Thursday AM — Room: 2022
February 19, 2009 — Location: Moscone West Convention Center

Session Chair: To Be Announced

8:30 AM

Control of Texture and Improvement of Magnetic Properties of Fe-6.5wt%Si by Directionally Recrystallization: Z. W. Zhang[1]; *G. Chen*[2]; H. Bei[3]; F. Ye[4]; G. L. Chen[5]; C. T. Liu[6]; E. P. George[6]; [1]Nanjing University of Science and Technology; [2]Nanjing University of Science and Technology, Oak Ridge National Laboratory; [3]Oak Ridge National Laboratory; [4]USTB; [5]Nanjing University of Science and Technology, USTB; [6]Oak Ridge National Laboratory and University of Tennessee

Fe-6.5%Si alloy is a high-silicon material with superior magnetic properties. However, it is difficult to be produced with controlled grain orientations by traditional processes. This research work reports for the first time that the grain orientation in the Fe-6.5%Si alloy can be controlled through directional recrystallization, and the coercivity force in the direction of 60°C along the growth direction of directional recrystallization can be reduced by 5 times than that without texture control. The significance of this work is that it not only makes it possible to produce grain-oriented Fe-Si alloys with high silicon content but also proves a unique way to control the orientation of magnetic materials magnetic property improvement. This work was supported by the Creative-Research-Foundation for PhD candidates of Jiangsu province, partially by the key project of China Natural Science Foundation (50431030) and by the U.S. Department of Energy, Materials Sciences and Technology Division.

8:50 AM

Electrodeposition of Ni-CNT Electrode Using Pulse-Reversal Current Technique: *Saleh Nowrouzi*[1]; Mehdi Attarchi[1]; S.K. Sadrnejad[1]; [1]Material and Energy Research Center

Ni electrode has been desired and applied by electrochemistry researchers because of its good properties. Several electrochemical applications of this material beside its good mechanical properties have persuaded to examine new methods of this material's synthesis. One of important electrochemical properties is surface area of this material which particularly is of great important in batteries. With co-deposition synthesis of Ni and carbon nano tubes (CNTs) it is possible to create nucleation centres on nanotubes and increase the surface area of Ni considerably. With pulse-reverse technique (PRC) which is an effective way to improve the performance of coating, co-deposition of these two materials better carried out. In this study with investigation of various parameters of PRC technique, the optimum statues of this technique are found out.

9:10 AM

Examination of Charge Transport Mechanisms in Vanadium Oxide Thin Films for Infrared Imaging: *Bharadwaja Srowthi*[1]; C. Venkatasubramanian[1]; N. Fieldhouse[1]; S. Ashok[1]; M. Ashok[1]; [1]The Pennsylvania State University

Current commercial uncooled infrared focal plane arrays rely on vanadium oxide (VO_x) thin films as the sensitive imaging layer. To date, however, very little is understood about the conduction mechanism that enables cameras to resolve temperature differentials approaching 10 mK. In this work, charge transport mechanisms in the VO_x films deposited using a pulse dc sputtering were analyzed in terms of band and hopping mechanisms. The resistivity and temperature coefficients of resistance values of the films varied between 0.1-100 ohm-and -1.1% to -2.4% K^{-1} respectively by varying composition *via* processing conditions. High temperature resistivity *vs.* temperature response of these films seems consistent with a band type conduction mechanism whereas, the origins of low temperature charge transport was due to charge hopping phenomena. These differences in electrical properties were due to variations in the density of states and statistical shift in the Fermi energy level due to temperature dependent disorder.

9:30 AM

Giant Magnetoresistance and Microstructure of CuCo Granular Prepared by Electrodeposition: *Zhao Lin*[1]; [1]Northeastern University

CuCo granular flims were prepared by electrodeposition on semiconductor Si. We studied the microstucture of the granular films during electrodepositing and elements distribution of the granular flim after annealing. The maximum value of GMR was obtained at Cu80Co20 flim after annealing at 450° for 1h, with increasing the temperature of annealing, the electrical resistivity was dropped. Surface scanning for elements analysis and XRD show that the separation of Co grain was occurred during annealing, and part Co-rich regions was appeared. It was contribution to improved the value of GMR by resistance measure.The value of the GMR was decreased after annealing at higher temperature.The saturation magnetiation Ms coercive forceHc remanence magnetization Mr were increased with improved the annealing temperature by magnetization measure.

9:50 AM Break

10:10 AM

Optical Properties of Molybdenum Oxide Thin Films Deposited by Chemical Vapor Transport of MoO3(OH)2: *Young Jung Lee*[1]; Hee Young Jeon[1]; Chang Won Park[1]; Dae-gun Kim[1]; Young Do Kim[1]; [1]Hanyang University

MoO3 thin films have been extensively investigated in the electrochromic (EC) device field due to its superior optical properties; electrochromism is simply defined as a color change caused by an applied bias. Recently, many deposition techniques to deposit Mo oxide thin films have been developed including chemical vapor deposition (CVD), evaporation, sol-gel coating, RF magnetron sputtering, and pulsed laser deposition (PLD). In this study, MoO2 thin films was homogeneously deposited by the chemical vapor transport (CVT) of MoO3(OH)2 during reduction of MoO3 powder in H2. Subsequently, a MoO3 thin film was obtained by annealing of the deposited MoO2 at 400°C for various holding times in O2. As annealing commenced, the optical transmittance of the films increased due to the crystallinity resulting from phase change and subsequent reduced oxygen vacancy.

10:30 AM

Study of Failure Mechanism by Electromigration in Au/Al Wire Bond: *Emil Zin*[1]; Nancy Michael[1]; S. H. Kang[2]; K.H. Oh[2]; U. Chul[3]; J. S. Cho[3]; J. T. Moon[3]; Choongun Kim[1]; [1]University of Texas at Arlington; [2]Seoul National University; [3]MK Electron Co. Ltd.

This study investigates the mechanism of contact failure in Au/Al wirebond under the influence of electromigration. Conventionally,wirebond failure has been largely attributed to the formation of intermetallic compounds that increases contact resistance by itself as well as through formation of voids. However, there is a growing concern in microelectrics that electromigration may impart added influence on the contact reliability because wires used in modern and future devices should carry high density current, enough to induce electromigration. In our study, electromigration reliability of Au/Al wirebond is conducted at varying temperature, current density and Au compositions. Our study finds that

electromigration do influence the failure mechanism, perhaps more significantly than was previously believed, and that it is affected by alloying elements. This paper present supporting evidences along with understanding made from the failure analysis.

10:50 AM

Synthesis and Characterization of Superparamagnetic Co and CoNi Particles: *Maitreyee Bhattacharya*[1]; M. Ghosh[1]; S.K. Das[1]; B. Mahato[1]; [1]National Metallurgical Laboratory

Magnetic nano particles are presently the object of intensive research for their interest from fundamental and technological point of view. The special magnetic properties of iron, cobalt, nickel and alloys find promising use in various applications. Magnetic nano particles Co and CoNi were prepared by the reduction of synthesized Co2NiO4 and Co3O4 nano particles. A homogenous carbonate precipitation method was adopted for the synthesis of Co2NiO4 and Co3O4 nanocrystalline particles. Hydrogen gas was used to study the reduction behavior of Co2NiO4 and Co3O4 in the temperature range 250-550°C. The characteristics and properties of the particles were studied by transmission electron microscopy, scanning electron microscopy, XRD and magnetic measurements by Vibration Sample Magnetometer. Co and CoNi nano particles show single domain at temperature >500°C. Hydrogen reduction using synthesized metal oxides is effective to obtain a superparamagnetic Co and CoNi powder. The process is novel and cheap to produce superparamagnetic particles.

11:10 AM

Ultraviolet Photoconductive Properties of ZnO Thin Film/Nanowell Grown by Using Atomic Layer Deposition: *Chia-Ling Lu*[1]; Chih Chen[1]; [1]National Chiao Tung University

Self-organized ZnO thin film/nanowells are grown on Si/glass substrates by using an anodic aluminum oxide template and atomic layer deposition (ALD) to deposit ZnO. By using ALD, the deposition temperature can be as low as room temperature and there is no need for metal catalysts or seed layers. The nanowells are highly ordered and grew perpendicularly to the Si/glass substrates. We controlled the morphology of ZnO nanowell arrays by modifying ALD deposition processes. The microstructure of the ZnO appears to be polycrystalline, with a grain size that increases with increasing number of deposited cycles. Because of its relevance in UV detector applications, the UV photoconductive properties of ZnO thin film/nanowells were investigated to obtain the best transformation efficiency. Results to be presented at the conference will include photoluminescence, SEM and TEM images, and UV photoconduction data for the ZnO thin film/ nanowell arrays will be presented in the conference.

11:30 AM

Properties of the Long-Term Ordered Semiconductors: *Sergei Pyshkin*[1]; John Ballato[2]; George Chumanov[2]; Michael Bass[3]; Giorgio Turri[3]; [1]Academy of Sciences; [2]Clemson University; [3]University of Central Florida

Periodical monitoring since 1960th of optical and mechanical properties of the chosen III-V and Si crystals shows that the stimuli for long-term improvement of crystal quality prevail over those which lead to its degradation due to intensification of heterogenic distribution of impurities and defects. Evolution of optical and mechanical properties partly presented at international conferences testifies that now in GaP doped by N, impurity is a regular element of the new crystal lattice - it increases the forbidden gap, and at relevant concentration and level of optical excitation creates a bound excitonic crystal. $CdIn_2S_4$, now having the perfect normal (instead of partly inversed) spinel crystal lattice, as well as GaP with evenly distributed impurities, dislocations, and increased microhardness demonstrate new stable and bright luminescent phenomena, including stimulated emission and "hot" luminescence at room temperature. Existing technologies help us to reproduce artificially these naturally ordered structures for application in optoelectronics.

General Abstracts: Materials Processing and Manufacturing Division: Session III

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: Surface Engineering Committee

Program Organizers: Thomas Bieler, Michigan State University; Neville Moody, Sandia National Laboratories

Thursday AM — Room: 3022
February 19, 2009 — Location: Moscone West Convention Center

Session Chair: To Be Announced

8:30 AM

Analysis of Anisotropy Behavior in UOE Forming for X80 HSLA Steel: *Sadegh Moeinifar*[1]; [1]Azad University

Anisotropy can potentially affect the integrity of the line pipes, such as their buckling and collapse resistance.Tensile and impact fracture toughness samples selected from 90 and 180° of pipe in longitudinal and transverse directions. The microstructures of the rolled plate have a fine acicular ferrite microstructure with some (M/A) that dispersed in the matrix phase.Tensile properties in 90° (transverse) are highest. Yield strength is about 6% higher that before UOE forming. Minimum amount of charpy impact appears in 90°(transverse) that amount of toughness decrease is about 5.5% in this orientation. Test temperature decrease from 0°C to -50°C show toughness impact energy decrease about 0.4-0.9% related to degree and orientation of samples. Therefore impact fracture toughness in all degree and orientation low dependent to decrease in temperature up to -50°C in X80 HSLA steel after UOE forming.

8:50 AM

Slurry Erosive Wear Behaviour of Laser Surface Alloyed 13Cr-4Ni Steel for Hydroturbine Applications: *R. C. Shivamurthy*[1]; M. Kamaraj[1]; R. Nagarajan[1]; S. M. Shariff[2]; G. Padmanabham[2]; [1]Indian Institute of Technology; [2]ARCI Hyderabad

13Cr-4Ni steels are extensively used as guide vanes, runners and nozzles in hydroturbine systems for power generation. These components normally found to undergo severe silt erosion during service. Laser surface modification with hardfacing alloys like Colmonoy 88 and Stellite 6 are proved to improve erosion resistance. In the present work, erosion behaviour of river sand is compared with commercial silica sand on laser surface alloyed steel at varying impact angles and constant slurry velocity. The erosion test result indicates that silica sand is found to be more aggressive in its erosion behaviour compared to river sand at all impact angles. The chemical analysis of erodents indicates that the river sand is an admixture of silica, alumina and several other oxides, where as commercial sand is pure silica. This indicates that the erosion rates are highly influenced by the volume fraction of hard silica particles within the erodent type.

9:10 AM

Effect of Al Contents on Recrystallization Kinetics of High Manganese Steel: *Hyuk-Jin An*[1]; Yang-Mo Koo[1]; Jae-Sang Lee[1]; Gyo-Sung Kim[2]; [1]Pohang University of Science & Technology; [2]POSCO Technical Laboratory

High Manganese steel is extensively studied for the application of high performance automotive steel. In this work, recrystallization kinetics of high-manganese steel was studied. To observe the kinetics of recrystallization of cold rolled specimen, Vickers hardness tests and microstructure observation were performed with varying Al contents and annealing condition, and Vickers hardness was analyzed by using the Avrami equation. The textures of hot rolled, cold rolled and fully re-crystallized specimen were analyzed by electron back scattering microscopy (EBSD). And the effects of Al contents on texture of high-manganese steel will be discussed.

9:30 AM

Effect of Small Additions of Boron on Shape Memory Properties and Grain Refinement of Cu-Al-Mn SMAs: *Sampath Vedamanickam*[1]; U.S. Mallik[2]; [1]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras; [2]Department of Mechanical Engineering, Siddaganga Institute of Technology

Cu-12.5wt.% Al-5.0wt.% Mn shape memory alloys with varying amounts of boron (0.05-0.2wt.%) were prepared by the casting route in an induction furnace under argon atmosphere. The Al and Mn contents of the alloys were maintained constant, while that of B was varied. The ingots obtained were homogenized followed by step quenching them to obtain a fully martensitic structure. The alloys were then characterized by subjecting them to compositional analysis, DSC and microstructural examination. The shape memory effect and superelasticity of the alloys were determined by bend and tensile tests. The study reveals that B acts as a good grain refiner, leading to a decrease in grain size of about 80%. Moreover, it increases the transformation temperatures by ~ 10°C, while at the same time decreasing the strain recovery by shape memory effect by 4%, and superelasticity by ~ 2%. Experimental results are presented and discussed in detail in this paper.

9:50 AM

Hydroxyapatite Coating on Titanium Using Induction Plasma Spray: Mangal Roy[1]; Amit Bandyopadhyay[1]; *Susmita Bose*[1]; [1]Washington State University

Plasma sprayed hydroxyapatite (HAp) coatings are widely used in orthopedic and dental applications. Most of these applications demand strong adhesion with the substrate and in vivo stability. To maintain long term stability, high level of crystallinity is necessary in HAp coatings, since resorption rate of amorphous HAp is significantly higher than its crystalline form. During plasma spray, partially melted particles dissipate heat to the substrate and cool at a very high rate. Rapid cooling increases amorphicity in HAp coatings. Therefore most of the coating at or near the interface is amorphous in nature. We have explored the influence of a thermal barrier layer to improve coating crystallinity. XRD results show that the surfaces of the coatings are highly crystalline with insignificant phase decomposition. The presentation will include interface microstructure, crystallinity, hardness, adhesive strength, flexural strength and wear properties of induction plasma spray HAp coatings on Ti substrate.

10:10 AM

Modeling Anisotropic Deformation of Tantalum Processed by Equal Channel Angular Pressing: *Michael Nixon*[1]; Joel House[1]; Philip Flater[1]; [1]Air Force Research Laboratory/Munitions Directorate

This study describes the computational modeling of the dynamic deformation of a commercially pure tantalum material after it was processed by equal channel angular pressing. Three variations were tested and simulated: as worked, fine-grain annealed, and large-grain annealed. Due to the processing, the materials display transverse isotropic behavior. Comparisons are shown between the well known Hill model of 1948 and a recent anisotropic description involving both the second and third invariants of the stress deviator. The test results also show a clear correlation between grain structure and macroscopic deformation that is captured by both models.

10:30 AM

Performance of Improved Autocatalytic Nickel Boron Coating System as a Potential Replacement for Chrome Plating in Aerospace Applications: *Kevin Garing*[1]; [1]Praxair Surface Technologies

There has long been interest in nickel boron plating, primarily because of unique deposit properties that generate a surface with good wear resistance and low coefficient of friction. The coating has found limited use due to the difficulties in maintaining the complex bath chemistry and poor performance against corrosion. This paper discusses a new, stabilized nickel boron process and its pairing with base coats and sealants for improved performance. The preferred morphology is identified and evaluated as a baseline, and then evaluated as part of a complete coating system that will provide lubricity, wear resistance, and corrosion protection. The link between tightly controlled process parameters, coating structure, and performance is demonstrated, and efforts to improve performance by changing the deposit morphology are discussed. A comparison to chrome and other coatings commonly used in low-friction and wear-resistant applications is provided along with a discussion of other potential uses.

10:50 AM

A Novel Process for Preparing Strontium Carbonate with Celestite Concentrate: *Mudan Liu*[1]; Tao Jiang[1]; Guanghui Li[1]; Guangzhou Qiu[1]; [1]Central South University

Preparation of high-purity strontium carbonate from celestite flotation concentrate by agglomeration-roasting process is studied. It is indicated that, by the results of SME and natural ballability analysis, celestite concentrates are difficult to agglomerate as they possess flat and silky surface, high viscosity and strong hydrophobicity. Lignin xanthate is added to improve the ballability, and the drop strength of green pellet is 7 times×(0.5m) -1 when the dosage is 0.5%. Roasting results show that the SrSO4 conversion of celestite pellet is 82~83%, which is 10% higher than celestite lump under the same conditions, as different structure causes different reaction kinetics conditions between them. The high-purity strontium carbonate with the SrCO3 content of 98.25% and CaCO3 content of 0.3% are obtained under the conditions of leaching temperature of 92° and time of 8h, carbonation temperature of 60° and time of 60min, ratio of NH4HCO3 and Sr(OH)2 of 1/1.

11:10 AM

Severe Deformation by Linear Flow Splitting of Low Alloyed Steels: *Enrico Bruder*[1]; Tilman Bohn[1]; Felix Rullmann[1]; Clemens Müller[1]; [1]TU Darmstadt

The innovative linear flow splitting process enables the continuous production of bifurcated profiles from plain sheet metal without lamination, joining of material or heating of the semi-finished product. The modified roll forming process uses obtuse angled splitting rolls and supporting rolls to form flanges out of the band edge which involves severe plastic deformation in the process zone. The necessary formability of the material is constituted by high hydrostatic compressive stresses, resulting in the formation of an ultrafine grained microstructure. Thereby a steady state is reached in the process zone where increasing deformation leads no more to significant changes in microstructure and mechanical properties. The present paper outlines for different low alloyed steels the evolution of linear flow split profiles by finite element simulation and by microstructural observations in the process zone.

11:30 AM

Surface Modification and Characterization of Commercially Available Nylon-6,6 Fibers for Electroless Nickel Deposition: *Gina Bunster*[1]; Jason Nadler[1]; [1]Georgia Tech Research Institute

An electroless nickel plating process has been developed that employs commercially available polymer fibers. Commonly experienced challenges are addressed in this work, which include finding a suitable polymer substrate, determining an effective etching method, and relating substrate surface area to the effectiveness of catalyst adsorption. Numerous studies testing the suitability of oxidizing and dissolution agents as etchants for nylon-6,6 (polyhexamethylene adiamide) resulted in the formulation of a 25 vol % 2-chlorophenol solution in toluene. Measurements of the resulting etched surface area were obtained using atomic force microscopy (AFM) in conjunction with quantitative image analysis. Etching increased exposed surface area and is correlated to the initial deposition rate of nickel.

11:50 AM

The Study of Droplet Impact Behavior on Different Surface Roughnesses: *KuZilati KuShaari*[1]; [1]Universiti Teknologi PETRONAS

The understanding of the behavior of a droplet impinging a flat surface is important in knowledge development in many engineering disciplines, such as spray coating, ink-jet printing and plasma coating. The focus of this work is to investigate the maximum spreading diameter or the spreading factor, of a single droplet on metal surfaces, namely stainless steel and etched silicon, having different surface roughnesses. A CCD high-speed camera with framing rate of 2,000, attached to a microscope, was used to capture the phenomena. The results of the stainless steel surfaces show that the rougher the surface the lower the spreading factor. All of the droplets on these surfaces also demonstrate that a droplet with a higher spreading factor gives a lower bouncing factor. However, the results of the etched silicon surfaces with the range of roughness used in this work, does not show a significant different in their spreading factors.

General Abstracts: Materials Processing and Manufacturing Division: Session IV

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: Surface Engineering Committee

Program Organizers: Thomas Bieler, Michigan State University; Neville Moody, Sandia National Laboratories

Thursday AM — Room: 3008
February 19, 2009 — Location: Moscone West Convention Center

Session Chair: To Be Announced

8:30 AM

Weldability of Advanced High Strength Steels (AHSS) Martensitic Type by Resistance Spot Welding (RSW): An Optimization Model to the Automotive Industry Components: Arturo Reyes-Valdes[1]; *Victor Lopez-Cortes*[1]; [1]Corporacion Mexicana de Investigacion en Materiales

When joining AHSS Martensitic Type with Resistance spot welding the correct welding schedule is an important production process part for successful assembly. Automotive manufacturers require optimized weld schedules that meet the customer quality requirements to obtain the best weld performance during the life vehicle. In certain instances modifications to welding parameters like current, pressure and time are made and the welding performance of the spot weld change and the mechanical and metallurgical properties are modified. This paper presents the results of the variables impact of Spot Welding Process in the weldability, welding metallurgy and quality characteristics of the AHSS Martensite Type welds. The microstructure, hardness and mechanical tensile properties were evaluated according with the different process condition. In order to know the multivariate correlation, a statistical and neural network models were obtained. A comparative study between these models was analyzed to apply at real condition.

8:50 AM

Changes in Microstructure and Mechanical Properties of CIP-Processed Tungsten Rods during Rotary-Swaging and Stretching Operations: Ismail Duman[1]; *Duygu Agaogullari*[1]; [1]Istanbul Technical University

The microstructure of the in rotary swagers hammered rods is gradually transformed from sintered to compact metallic. In order to gain a high quality product, it is essential to optimize the wire draft production conditions and to control the recrystallization (inductive annealing) process particularly. Tensile strength of swaged rods (wire drafts) is determinative for the next step i.e. stretching by turn-tables. In this study, as a part of the complete process for thin wire ($\phi < 10$ micron) production, changes in microstructure (grain size and grain population density) and mechanical properties (density, porosity, hardness and tensile strength) during swaging and stretching of tungsten to 400 micron are investigated. The mentioned wire is obtained using industrial scale equipments by passing the rod (ϕ 16 mm) through three rotary-swagers (ϕ 7.6 mm, 4 mm, 3 mm respectively), intermediate annealing (2400°C) and through three stretching machines (turn-tables) each with H_2/N_2 protected heating furnaces.

9:10 AM

Dynamic Recrystallization Texture in Nickel Superalloys 718 and 718plus: *James Baird*[1]; Haitham El Kadiri[1]; Hongjoo Rhee[1]; Abel Lowry[1]; Mark Horstemeyer[1]; Paul Wang[1]; [1]The Center for Advanced Vehicular Systems

We studied the effect of dynamic recrystallization on the deformation texture generated by simple compression in two grades of Nickel super alloy; 718 and 718plus. The texture was analyzed through Electron Backscattered Diffraction (EBSD) technique. The Compression tests were carried out on cylindrical and double cone samples at three different temperatures, two different strain rates and several dwelling times after deformation. The double cone compression tests were performed to examine the effect of a strain gradient on texture. The dynamic recrystallization showed different trends for the two alloys and induced a quite different texture through deformation.

9:30 AM

Effect of Si/Mg Molar Ratio on the Electrochemical Behavior of Al/SiCP Composites with Bimodal Distribution of Reinforcements: *Miguel Montoya-Dávila*[1]; Martin Pech-Canul[1]; Maximo Pech-Canul[2]; [1]Cinvestav-Saltillo; [2]Cinvestav-Mérida

The effect of the Si/Mg molar ratio - in the raw aluminum alloy - on the electrochemical behavior of Al/SiCp composites was investigated. Composites were fabricated by reactive infiltration of porous preforms with 0.6volume fraction of silica-coated SiC with particle sizes of 10 and 146 µm, in the particle size ratio 1:5, correspondingly. Four experimental Al-Mg-Si alloys with Si/Mg molar ratios of 0.12, 0.49, 0.89, and 1.05, were used to infiltrate the preforms in argon followed by nitrogen, at 1100ºC for 60 min. The composites were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM) before and after electrochemical tests, measuring the corrosion potential (Ecorr) and cyclic polarization in aerated and de-aerated 0.1M NaCl solutions, respectively. Results show that pitting potential (Epit) becomes less negative with decrease in the Si/Mg molar ratio, thus enhancing the corrosion resistance. By contrast, Ecorr tends to similar values after two hours of immersion.

9:50 AM

Functionally Graded Boron Carbide and Aluminum Composites with Tubular Geometries Using Pulsed Electric Current Sintering: *Troy Holland*[1]; Dustin Hulbert[2]; Amiya Mukherjee[1]; [1]University of California, Davis; [2]Nanosolar, Inc.

Functionally graded boron carbide (B4C) with precipitous property and microstructural gradients has been synthesized using pulsed electric current sintering (PECS) in tubular shape forms. This processing route results in a material with very promising inner diameter properties while blending smoothly into those of cast aluminums on the outside. During PECS the amorphous powders react and partially consolidate forming a density gradient. Modeling results support the presence of a large radial temperature gradient sufficient to produce B4C in smoothly varying densities from inside to outside. This material and geometry is both novel and of particular use in applications requiring a cylinder of differing surface structures that transition smoothly into a metallic substructure or assembly.

10:10 AM

Hybrid Monte Carlo/Vertex Simulation of Strain-Induced Grain Growth: *Corentin Guebels*[1]; Benjamin Fell[1]; Tien Tran[1]; Joanna Groza[1]; Jean-pierre Delplanque[1]; [1]University of California

The prediction of microstructural evolution and abnormal grain growth phenomena during high-temperature creep requires an accurate description of recrystallization. A two dimensional Monte Carlo - Vertex (MC-V) model is presented which characterizes grain-growth kinetics during strain-induced recrystallization. The MC-V model presents a powerful means to incorporate strain affects into Monte Carlo grain growth simulations. The current approach tracks strain-induced microstructural phenomena at grain boundary junctions, as well as within the grain, to capture grain sliding and rotation events, diffusion along grain boundaries, and plastic work. By capturing these realistic geometrical constraints, combined with a dynamically reorganizing numerical lattice, the model provides a flexible, physics-based methodology to investigate external influences on the microstructural evolution. The simulation results clarify the influences of deforming microstructure on grain growth kinetics.

10:30 AM

Model of Thermal Physics in Plasma-Sprayed Coatings and Calculation of Residual Stress: *Liping Niu*[1]; Ting-an Zhang[1]; Jicheng He[1]; Zhihe Dou[1]; Yan Liu[1]; Guanyong Shi[1]; Xiaochang Cao[1]; [1]Northeastern University

Different thermophysical properties of the substrate and coating materials and different spraying parameters deduce the residual internal stress induced in thermally-sprayed coating composite materials during deposition. In this paper, thermal physic model of temperature field at the plasma spraying processe based on analysis of particle's deposition process is established. Spraying process parameters and mechanical and thermal properties of sprayed materials are considered. Regarding the formation of coating as superimposed n sub - coatings with thickness hmin, the change of temperature can be described by a two-step calculation model: at the initial step temperature doesn't exceed 20% corresponding spraying material melting point; at the final step substrate and coating are bound and led to the formation of residual stress when both of them achiave the highest temperature of system. This model has made it possible to evaluate the components of residual stresses.

10:50 AM
Residual Stress Reduction for Air Plasma Sprayed Al-Si Abradable Coating: *Jon Tucker*[1]; Terry Alford[1]; [1]School of Materials, Arizona State University

Air plasma spray is a common process used to apply abradable coatings. However the large residual stresses make the layers prone to delamination. Therefore it is important to elucidate the mechanisms of the high residual stresses. To determine an effective method to reduce the residual stresses present in the coating, heat treatments were preformed to better understand the effects that a post-deposition heat treatment has on the microstructure and subsequent stress levels in the abradable coating. The microstructure and stress analyses included x-ray diffraction, energy dispersive x-ray spectroscopy, and secondary electron microscopy. Analysis of the microstructure and residual stress of the heat treated samples revealed that a key factor in the reduction of residual stress is formation of silicon precipitates.

11:10 AM
Porous NiTi Shape Memory Alloy Structures Using Laser Engineered Net Shaping: Vamsi Balla[1]; Susmita Bose[1]; *Amit Bandyopadhyay*[1]; [1]Washington State University

Porous NiTi alloy samples were fabricated with 12 to 36% porosity from equiatomic NiTi alloy powder using Laser Engineered Net Shaping (LENS). LENS processed porous NiTi samples showed high amount of cubic B2 phase compared to feed stock powder. Moreover, high cooling rates associated with laser processing increased the reverse transformation temperature due to thermally induced stresses and defects. Transformation temperatures were found to be independent of pore volume, while high pore volume in the samples decreased the maximum recoverable strain from 6% to 4%. Porous NiTi samples with 12 to 36% porosity exhibited low Young's modulus between 2 and 18 GPa as well as high compressive strength and recoverable strain. These porous samples are thus promising biomaterials for different applications including hard tissue replacements. This talk will focus on process-structure-property correlation of these porous NiTi alloy samples.

11:30 AM
Surface Hardening of Titanium and Ti-6Al-4V Using near- Atmospheric Pressure Plasma Generated by CO2 Laser Irradiation: *Ravindra Kumar Akarapu*[1]; Dana Scott[1]; Abdalla Nassar[1]; Stephen Copley[1]; Judith Todd[1]; [1]Penn State University

Titanium and its alloys are widely used in the aerospace industry due to their high specific strength and good corrosion resistance. Tribological coatings may be required for high wear resistance applications. Surface coating processes such as plasma nitriding or chemical vapor deposition (CVD) require vacuum environments and yield low coverage rates. This paper discusses a near-atmospheric pressure surface hardening process, developed using plasma generated by CO2 laser irradiation of titanium and Ti-6Al-4V alloy in the presence of shielding gas mixtures (Ar + N2, Ar + CO2) to yield nitrides, oxynitrides and oxycarbides. The effect of mole fraction of Ar on the active species in the plasma was studied by optical emission spectroscopy. Optimized parameters for deposition of near-stoichiometric titanium nitride will be discussed.

11:50 AM
The Structure and Properties of Glass-Coated Amorphous FeCoSiB Micro-Wire: *Zhihao Zhang*[1]; Chengduo Wang[1]; Fengmei Wang[1]; Jianxin Xie[2]; [1]Advanced Materials and Technologies Institute, University of Science and Technology Beijing; [2]State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing

Because of the excellent performance, glass-coated amorphous metallic micro-wires get comprehensive application in many regions, such as sensor devices, forgery prevention label and electromagnetic shielding materials. In this paper, the glass-coated Fe69Co10Si8B13 amorphous micro-wires with various glass coating thickness and metallic core diameter are fabricated through adjusting casting rate and cooling water position. The relationships between the microstructure and mechanical properties of the micro-wire with casting rate, cooling condition and annealing process are analyzed. The critical casting rate for preparing amorphous micro-wire is determined. The influences of the ratio between core diameter and coating thickness as well as the annealing process on the remanence ratic, coercive force and large Barkhausen effect are investigated.

Magnesium Technology 2009: Modeling

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

Thursday AM — Room: 2006
February 19, 2009 — Location: Moscone West Convention Center

Session Chairs: Eric Nyberg, Pacific Northwest National Laboratory; Sean Agnew, University of Virginia

8:30 AM Introductory Comments

8:35 AM
Blind Study of the Effect of Processing History on the Constitutive Behavior of Alloy AZ31B: *Cyrus Dreyer*[1]; F. Polesak[1]; Thomas Shultz[2]; Sean Agnew[1]; [1]University of Virginia; [2]Hampden-Sydney College

The discipline of materials science is founded upon the structure-property paradigm, and yet it is often held that the full processing history must be known in order to predict material properties. The latter is in conflict with the fundamental premise. The present study probes these philosophical issues within the context of a blind study of AZ31B sheet tensile properties. Four sheets were processed by different vendors and by different approaches, including strip casting and more conventional direct chill ingot casting followed by hot rolling. The experimentalists do not know which sheets were subjected to a given processing history. Property distinctions between the sheets, such as flow strengths, anisotropies, and propensities for dynamic recrystallization and cavitation, are explained in terms of observable structural quantities: grain size and shape, texture, and particle distributions. The results provide sheet producers with microstructure guidelines to augment current property targets.

8:55 AM
New Microalloyed Magnesium with Exceptional Mechanical Performance: *Anja Hänzi*[1]; Timo Ebeling[2]; Rüdiger Bormann[2]; Peter Uggowitzer[1]; [1]ETH Zürich; [2]Hamburg University of Technology

New Mg–Zn alloys have been developed according to the microalloying concept and in consideration of growth restriction during alloy casting and forming. After extrusion (30:1) they reveal very fine grains (< 10 µm), excellent ductility (uniform elongation: 17-20%) at considerable strength (UTS: 250-270 MPa) and homogeneous distribution of intermetallic particles, which suppress grain growth even at comparably high temperatures. The new alloys exhibit also very low tension-compression asymmetry ($R_{p,tension}$ / $R_{p,compression}$ ~ 1). This phenomenon is not only ascribed to the weak texture but also to the fine-grained structure, which enables activation of complimentary deformation processes (non-basal slip) at RT. Indeed, simulations of the deformation modes indicate very soft prismatic slip. Furthermore they explicitly point to activation of tension twinning {10-12}<10-11>, which is rather unusual for fine-grained Mg alloys. Due to the choice of only biocompatible alloying elements, the new alloys are very promising for applications in a broad range.

9:15 AM
A New Approach for Inverse Parameter Calculations of the Plastic Deformation Behavior of AZ31 Magnesium Alloy: *Timo Ebeling*[1]; Christian Hartig[1]; Rüdiger Bormann[1]; [1]Hamburg University of Technology

In order to improve the mechanical properties of magnesium wrought alloys, a better understanding of the texture evolution and anisotropic behavior is necessarily needed. The approach is a detailed investigation of the deformation mechanisms by model calculations. Therefore, room temperature tensile tests of AZ31 hot rolled sheets have been performed and the stress-strain behavior as well as the r-value-function has been measured. An inverse parameter calculation yielding information about deformation mode activities, texture evolution and mechanical properties was performed using a viscoplastic self-consistent model. The first objective function of the inverse parameter calculation was the macroscopic hardening. Additionally the r-value, which reacts strongly on changes of the yield surface, was introduced into the modeling as a second objective function. The additional input of experimental r-values can result in a better understanding of the mostly disregarded latent hardening of the deformation modes.

9:35 AM

Dislocations and Their Configurations in Mg and Mg Alloys: *Bin Li*[1]; Evan Ma[1]; K. T. Ramesh[1]; [1]Johns Hopkins University

Mg and Mg alloys have attracted significant attention in recent years. Despite extensive investigations on the deformation mechanisms in Mg over the past several decades, specifics of dislocation slip during deformation remains controversial, partly due to the complicated slip systems. There are three possible Burgers vectors that differ significantly in magnitude, <a>, <c> and <c+a>, and the identification of the dislocations by TEM is not trivial. Consequently, there are misunderstandings and misinterpretations about the dislocations in Mg and Mg alloys, especially the <c+a> dislocation for pyramidal slip. We present TEM observations on the dislocations and stacking faults in deformed Mg and Mg alloys with various plastic strain levels (2%, 4% and 8%). We show that using an appropriate zone axis <01-10> and the weak-beam-dark-field (WBDF) technique, we can determine the Burgers vectors of the dislocations with clarity. We also show TEM observations of the <c+a> dislocations and the stacking faults.

9:55 AM

Lattice Reconstruction – A Crystallographic Model for Grain Reorientation in HCP Magnesium: *Bin Li*[1]; Evan Ma[1]; [1]Johns Hopkins University

We present a new model to describe the crystallographic reorientation in HCP Mg during deformation. In this model, the original lattice can be reoriented by 90 degrees, by reconstructing new basal planes from the existing lattice points on the {10-10} prismatic planes, such that the new basal planes are parallel to the loading axis (possibly also relevant to texture formation in deformed polycrystalline Mg). The structural deviation between the original and the new lattices is so small (much shorter than any known Burgers vectors) that it can be accommodated by a simple shear. We show that this minor structural deviation can be compensated by either elastic shear strain or plastic strain to establish the correct stacking sequence. Molecular dynamics simulations are performed to investigate the mechanism of lattice reorientation in single crystal Mg during shear and tensile deformation.

10:15 AM Break

10:30 AM

Microstructural Investigation of Twins under the Fracture Surface in AZ31 Mg Alloys: *Daisuke Ando*[1]; Junichi Koike[1]; [1]Tohoku University, Department of Materials Science

Magnesium alloys form many types of twins which play important roles on deformation and failure. Reed-Hill and others suggested that double twins are the origin of poor ductility. Recently, we experimentally showed that double twins accompany large surface relieves and cracks. However, the current knowledge does not provide an undisputable evidence of the double twins being the major reason for premature failure. In this work, we performed detailed observation and analysis of the underlying microstructure on fractured surface. The sample was a rolled AZ31 sheet. Tensile test was performed at room temperature. A number of facets were observed on fractured surface. Cross-sectional TEM samples were prepared by FIB from these facets. TEM observation showed the formation of double twins underneath the facet. The presence of fine recyrstallized grains indicates substantial dislocation activity related to the double twins. These results indicate the relation between localized large deformation and macroscopically brittle failure.

10:50 AM

Mechanisms of Deformation and In Situ 3D Damage Analyses during High Temperature Deformation of an AZ31 Mg Alloy: *Jean-Jacques Blandin*[1]; Luc Salvo[1]; Remi Boissiere[1]; Jerome Adrien[2]; Eric Maire[2]; [1]Grenoble Institute of Technology; [2]INSA Lyon

Large elongations to fracture (> 300%) can be obtained during high temperature deformation of the AZ31 Mg alloy. This capacity results from the ability to activate deformation mechanisms displaying a high value of the strain rate sensitivity parameter and from the resistance to strain induced damage. In this work, the effect of strain rate and temperature on the rheology of a fine grained AZ31 alloy was investigated and experimental domains for which a high plastic stability is expected were identified. A particular attention was also given to the quantification of damage during high temperature deformation. A 3D damage characterisation was performed thanks to the use of X-ray microtomography for imaging the cavities. Post mortem investigations were performed but an in situ characterisation was also attempted thanks to a specifically dedicated device allowing concomitant high temperature deformation and fast acquisition X-ray micro tomography analysis.

11:10 AM

New Crystal Plasticity Constitutive Model for Large Strain Phenomena in HCP Metals: *Adel Izadbakhsh*[1]; Kaan Inal[1]; Raja Mishra[2]; Sanjeev Bedi[1]; [1]University of Waterloo; [2]General Motors

Secondary twinning systems are important deformation mechanisms in pure magnesium and its alloys. For a given texture of these metals in certain loading paths, these microscopic deformation mechanisms account for a significant amount of macroscopic strain. The existing crystal plasticity based constitutive models do not account for the kinematics of these deformation mechanisms. To address this limitation, a crystal plasticity based constitutive model that individually simulates the slip-induced shear in the matrix, primary and secondary twinned regions, and twin-induced shear in the primary and secondary twinned regions has been developed for Hexagonal Closed-Packed (HCP) metals. Separate resistance evolution functions for the primary, secondary, and tertiary slip systems, as well as primary and secondary twinning systems have been considered. The model tracks the texture evolution in the matrix, primary, and secondary twinned regions. Numerical simulations have been performed for HCP single crystals and the effects of model parameters have been investigated.

11:30 AM

Application of a Finite Strain Elastic-Plastic Self-Consistent Model to Deformation of Magnesium: *Bjørn Clausen*[1]; C Neil[2]; Sean Agnew[2]; Donald Brown[1]; Carlos Tomé[1]; [1]Los Alamos National Laboratory; [2]University of Virginia

The traditional elastic-plastic self-consistent (EPSC) model, which is a small strain formulation that does not take into account lattice rotations, has been applied with great success to simulations of metals at low degrees of plastic deformation. The application of the EPSC model to low symmetry materials, such as magnesium, is only approximate as texture evolution due to both slip and twinning can be pronounced even in the early stages of plastic deformation. Recently, a finite strain version of the EPSC model has been developed which includes grain reorientation due to twinning and slip. With the new finite strain model in hand, we can now account for the effect of slip and twinning reorientation upon the evolution of internal stress and peak intensities during plastic deformation. The new model has been used to explain the observed texture and internal stress changes measured in-situ using neutron diffraction during compressive loading of extruded magnesium.

11:50 AM

Test Results and FEA Predictions from Magnesium AM30 Extruded Beams: *David Wagner*[1]; Steve Logan[2]; Kathy Wang[3]; Tim Skszek[4]; Christopher Salisbury[5]; [1]Ford Motor Company; [2]Chrysler LLC; [3]General Motors Corp; [4]Cosma International; [5]University of Waterloo

Load versus displacement measurements are compared to finite element analysis (FEA) predictions of the component behavior of magnesium AM30 extruded beams. Results from quasi-static four-point bend, quasi-static axial crush and high-speed axial crush tests of extruded magnesium AM30 beams show the beam's behavior over a range of loadings and responses. The extrude AM30 beams showed significant cracking and splitting in the tests. LS-DYNA material model MAT124 captures the extruded magnesium AM30 constitutive behavior over a range of strain rates and accommodates different responses in tension and compression. Examinations of various element sizes and failure criterion show the sensitivity and robustness of the predicted beam behavior. 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.

Materials for High Temperature Applications: Next Generation Superalloys and Beyond: Ceramic Composites and Other Technologies

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS: High Temperature Alloys Committee, TMS: Refractory Metals Committee
Program Organizers: Joseph Rigney, GE Aviation; Omer Dogan, National Energy Technology Laboratory; Donna Ballard, Air Force Research Laboratory; Shiela Woodard, Pratt & Whitney

Thursday AM — Room: 3010
February 19, 2009 — Location: Moscone West Convention Center

Session Chairs: Michael Cinibulk, Air Force Research Laboratory; Donna Ballard, Air Force Research Laboratory

8:30 AM Invited
Ceramic Composites Development for Air and Space Applications: *Michael Cinibulk*[1]; [1]Air Force Research Laboratory

Constant demands of greater high-temperature chemical and environmental stability, mechanical performance, durability, service life, and affordability continue to be made on materials systems for air and space applications. Next generation turbine and space propulsion systems continue to require higher operating pressures and temperatures, which require higher performing materials and systems than are currently available. Ceramics, both monoliths and composites, have achieved the level of development that is enabling their use as components in the combustor, turbine, and exhaust sections of demonstration turbine engines. However, their durability to ensure long life in actual production systems is lacking. Current thermal protection systems are projected to greatly limit the readiness and potential of "aircraft-like capabilities" of future reusable space launch vehicles; but, again, improvements in durability of the friable materials upon which these systems are based is required. The desire for aerospace vehicles to operate at hypersonic speeds is dependent upon dramatic improvements in high-temperature ceramics. This presentation will summarize work on ceramics development being targeted for air and space applications. A brief review of the recent research that is being conducted in our laboratory will also be provided.

8:55 AM
A Study on Flow Behaviors of Alloy IC10 over a Wide Range of Temperatures and Strain Rates: Hongjian Zhang[1]; Weidong Wen[1]; *Haitao Cui*[1]; Ying Xu[1]; [1]Nanjing University of Aeronautics and Astronautics

IC10 is a newly developed Ni3Al-based superalloy, with its nominal composition(wt%):0.07-0.12%C11.5-12.5%Co6.5-7.5%Cr5.6-6.2%Al4.8-5.2%W1.0-2.0%Mo6.5-7.5%Ta1.3-1.7%Hf0.01-0.02%B and Bal.Ni. To investigate flow behaviors of IC10, tensile experiments were conducted over a wide range of temperatures(293~1073K) and strain rates(0.00001~0.01/s) on Material Test System. Experiments show that:(1)flow behaviors are not sensitive to strain rates over the wide range of temperatures;(2)flow behaviors varies slightly with the temperature at the same strain rate. Z-A model, one of the most widely used models, is employed in describing the flow features of IC10. Normally, the parameters in Z-A model are regarded as constants in whole deforming process, which isn't agree with the actual process and will decrease its predicted accuracies. In order to improve the predicted accuracies, the parameters in Z-A model are modified by introducing the evolution function. The modified model is used to predict flow behaviors of IC10 under different experiment conditions. The results show that it is valid.

9:15 AM
A TEM Study of the Evolution of Deformation Mechanisms Following LCF of a Ni-Base Superalloy: *Patrick Phillips*[1]; Raymond Unocic[1]; Libor Kovarik[1]; Michael Mills[1]; [1]Ohio State University

The effect of microstructure on the high temperature low cycle fatigue deformation mechanisms of an advanced Ni-base disk superalloy was studied using TEM characterization methods. In order to track the evolution of these mechanisms, specimens were interrupted after a limited number of cycles and were not run to failure. Both fine and coarse precipitate microstructures were examined, corresponding to a fast or slow cool, respectively, from the gamma prime solvus temperature. Various microstructural attributes, such as smooth or serrated grain boundaries and precipitate size scale and morphology were correlated with the operative deformation mechanisms, which included stacking faults, dislocation bands, and microtwins. The evolution of the operative mechanisms with number of cycles will also be discussed.

9:35 AM
Advances in Non-Contact Measurement of Creep Properties: *Robert Hyers*[1]; Stacy Canepari[1]; Erica Bischoff White[1]; Laurent Cretegny[2]; Jan Rogers[3]; [1]University of Massachusetts; [2]General Electric Co; [3]NASA MSFC

As the required service temperatures for superalloys increases, so do the demands on testing for development of these alloys. Non-contact measurement of creep of refractory metals using electrostatic levitation has been demonstrated at temperatures up to 2300 C using samples of only 20-40 mg. These measurements load the spherical specimen by inertial forces due to rapid rotation. However, the first measurements relied on photon pressure to accelerate the samples to the high rotational rates of thousands of rotations per second, limiting the applicability to low stresses and high temperatures. Recent advances in this area extend this measurement to higher stresses and lower-temperatures through the use of an induction motor to drive the sample to such high rotational speeds. Preliminary results on new measurements on new materials will be presented.

9:55 AM
Study of Precious Metal Modified Ni-Based Superalloys Using the Calphad Approach: *Fan Zhang*[1]; Shuanglin Chen[1]; Weisheng Cao[1]; Ying Yang[1]; Kaisheng Wu[1]; Y. Chang[2]; [1]CompuTherm LLC; [2]University of Wisconsin

Precious metal modified nickel-based super alloys have recently been under development due to their excellent properties of high temperature oxidation and hot corrosion resistance. To improve the performance of precious metal modified nickel-based superalloys, alloy composition need to be carefully adjusted to promote the formation of desired phases and microstructure, while avoiding the formation of deleterious phases. This requires detail knowledge of phase equilibria in the multi-component nickel-based alloy systems. In this study, Calphad approach is used to develop a multi-component thermodynamic database which contains Pt, Ir and Ru. Using this database, effects of a variety of alloying elements on the materials properties, such as liquidus, solidus, gamma_prime solvus, gamma_prime phase fraction, elemental partitioning, and so on, can be predicted. Such information provides valuable guidance in the design and development of nickel-based superalloys. In this presentation, calculated results for a wide range of compositions will be discussed.

10:15 AM Break

10:25 AM
Exploring the 3D Nanospace of Defects Formed in Ni-Based Superalloys Using Atom-Probe Tomography Assisted by Dual-Beam Focused Ion-Beam Microscopy: *Yaron Amouyal*[1]; David Seidman[1]; [1]Northwestern University

Chains of misoriented grains are common defects occurring during the directional solidification of nickel-based superalloy single-crystals used for turbine blades in jet engines. These so-called freckles cause degradation in a turbine blade's mechanical properties at high-temperatures. Eliminating the formation of freckles is a compelling technological challenge, which can be achieved by characterizing an alloy's microstructure and composition at the micrometer to nanometer length scales. Transmission and scanning electron microscopic observations of multi-component (>10 elements) Ni-based superalloys reveal a microstructure comprising dendritic and inter-dendritic regions that are present in both the freckles and single-crystalline matrix. All four regions differ in their compositions. We employ the lift-out technique in the dual-beam focused ion-beam (FIB) microscope to prepare selectively samples for APT analyses in the form of sharply pointed tips (edge radius < 50 nm). Thus, we determine the roles played by different alloying elements in the formation of freckles.

10:45 AM
Development of Heat Treatment for a Powder Metallurgy Nickel-Base Superalloy: *Gaofeng Tian*[1]; Chengchang Jia[1]; Fazhang Yin[1]; Benfu Hu[1]; [1]University of Science and Technology Beijing

Nickel-base superalloys should have excellent high temperature performance to challenge the improved operating temperatures in advanced aircraft engines. An important approach to meet this goal to modify the heat treatment for these alloys, this could control the characteristic microstructures including grain size and the distribution of gamma prime phases, and hence, determine the mechanical properties. In this study, a new heat treatment was developed for

a powder metallurgy nickel-base superalloy, mechanical property testing was performed to assess the new heat treatment. The results of this investigation have shown that the new heat treatment can obviously improve the high temperature plasticity without sacrificing strength: elongation increases 33%, reduction in area increases 57%.

11:05 AM

Application of Advanced Creep Modeling Incorporating Damage to Nickel Based Superalloy: Nicola Bonora[1]; *Luca Esposito*[1]; [1]University of Cassino

The increasing demand of reliable creep design for longer lives requires model formulation in which the contribution of different creep and damage mechanisms should be accounted for. Recently, the authors (Bonora and Esposito, Proc. of ASMEPVP, 2008) proposed a creep model which takes into account the resulting action of both diffusional and dislocation type creep and damage effects associated with microvoids/cracks. In this work, the model has been extended to nickel-based superalloy. The following features has been addressed: a) the possibility to accurately predict the minimum creep rate over a wide range of stress/temperature; b) the extension to primary creep stage; c) the extension to damage mechanisms associated with microstructural changes that may occurs during long term high temperature exposure. The model has been implemented into FEM code and used to predict creep response of laboratory samples and components. Model application examples to MAR and Rene nickel-based superalloys are presented.

11:25 AM

Effects of Cr on the Stress Rupture of Ni-Based Single Crystal Superalloys: J. Y. Chen[1]; B. Zhao[1]; L. M. Cao[2]; *Qiang Feng*[1]; [1]University of Science & Technology Beijing; [2]Beijing Institute of Aeronautical Materials

Chromium is beneficial to hot corrosion resistance and oxidation resistance of Ni-based superalloys. However, Cr additions significantly promote the formation of TCP phases and degrade mechanical properties. In the current study, single crystal superalloys with various levels of Cr-additions (0~5.7wt.%) were investigated. It is very interesting to note that the Cr addition significantly improved the life of stress rupture at 1100°/140MPa from 30h in the Cr-free alloy to 138h in the alloy containing high levels of Cr additions. Meantime, the γ' morphology changed from spherical to cuboidal with the decrease of the precipitate size, and the volume fraction of γ' precipitates increased with increasing Cr additions. In order to understand the strengthening mechanism under the influence of Cr additions, the investigations on microstructure, partitioning behaviour of alloying elements, lattice misfit and stress rupture properties will be conducted, and the relationship among them will be discussed.

11:45 AM

Microstructure and Mechanical Properties of Directionally Solidified Castings Processed by HRS and LMC: Wenshu Tang[1]; Shen Jian[1]; *Jian Zhang*[1]; Langhong Lou[1]; Dawei Wang[1]; [1]Institute of Metal Research, Chinese Academy of Sciences

Large castings were directionally solidified (DS) using high rate solidification (HRS) and liquid metal cooling (LMC) techniques. The as cast microstructural features such as primary dendrite arm spacing, and size and fraction of eutectic and porosity were characterized as a function of the distance from casting chill. The heat treatment was also studied according to the measured incipient melting points. Room temperature tensile properties, creep rupture as well as low cycle fatigue properties of specimens sectioned at different position of the large castings were examined. Microstructure and mechanical properties of alloys with deliberately added Sn were also studied.A much finer and more homogenous structure along the DS direction was achieved by LMC process. A higher fraction of residual eutectics was found in HRS samples after heat treatment. No properties degradation was found in the present DS alloy containing up to 1200ppm Sn addition.

Materials for the Nuclear Renaissance: Materials: Manufacturing and Testing

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS/ASM: Corrosion and Environmental Effects Committee, TMS/ASM: Nuclear Materials Committee, TMS: Refractory Metals Committee

Program Organizers: Raul Rebak, GE Global Research; Robert Hanrahan, National Nuclear Security Administration; Brian Cockeram, Bechtel-Bettis Inc

Thursday AM — Room: 2009
February 19, 2009 — Location: Moscone West Convention Center

Session Chairs: Raul Rebak, GE Global Research; Brian Cockeram, Bechtel-Bettis Inc

8:30 AM

The Fracture Toughness and Toughening Mechanism of Commercially Available Unalloyed Molybdenum and ODS Molybdenum with an Equiaxed, Large Grain Structure: *Brian Cockeram*[1]; A. Mueller[1]; [1]Bechtel Bettis Inc

Commercially available molybdenum and ODS molybdenum produced by Powder Metallurgy (PM) methods are subject to fracture toughness testing and examination of the toughening mechanism. Both PM molybdenum and ODS molybdenum are shown to have an equiaxed grain size that is larger in scale than wrought products. Although the grain size for PM molybdenum is large and the oxygen content is relatively high, and these attributes tend to embrittle molybdenum, the transition temperature and fracture toughness values are comparable to those for wrought molybdenum. Crack initiation at grain boundaries and the center of grains where pores are present was observed to leave ligaments for the PM molybdenum that are similar in size to those observed for wrought molybdenum. This is a similar toughening mechanism to the ductile laminate mechanism observed for wrought molybdenum. The impact of grain size, grain shape, and oxide particles on the toughening mechanism and properties is discussed.

8:50 AM

Powder Diffraction Characterization of Reactor Materials: *Heather Volz*[1]; Christopher Stanek[1]; Samantha Yates[1]; Erik Luther[1]; John Dunwoody[1]; Kenneth McClellan[1]; Sven Vogel[1]; Sally Tracy[1]; [1]Los Alamos National Laboratory

Characterization studies of materials are important to many aspects of nuclear energy research. In this talk, an overview of recent work will be presented with a focus on powder diffraction studies as validation of UO_2 defect modeling. As an example from transmutation fuel development associated with closing the fuel cycle, changes in the lattice parameter due to lanthanide impurities in the UO_2 crystal structure may be related to cracking during the sintering process. Therefore, samples were prepared with various lanthanides in differing concentrations to validate atomistic simulations of various defect mechanisms in UO_2. Preliminary laboratory X-ray diffraction data show differences in lattice parameters as a function of lanthanide concentration that suggest the creation of U^{5+} ions predominate in Ln:UO2, contracting the unit cell. Time-of-flight neutron data from HIPPO at LANSCE's Lujan Center were also collected, and will be discussed.

9:10 AM

Microstructural Evolution and Multi-Scale Characterization of Sintered ZrN as a Surrogate for PuN Fuel Pellets: *Kirk Wheeler*[1]; Pedro Peralta[1]; [1]Arizona State University

ZrN was studied as a possible surrogate for PuN under the Global Nuclear Energy Partnership (GNEP) program. The mechanical properties of sintered ZrN pellets were examined at elevated temperatures to investigate the effects that sintering temperatures and post-sintering heat treatments have on structural integrity. Uniaxial compression testing was performed on ZrN pellets in a gettered ultra-high purity Argon atmosphere at various temperatures (25°C, 800°C, 1200°C). Post-Mortem fractography was performed using scanning electron microscopy (SEM). In addition, nano-indentation and nano-compression testing was performed on ZrN as well as nano-pillars that were produced using Focused Ion Beam milling. The failure modes of the pellets and their mechanical properties are evaluated in terms of the initial microstructure. Applicability of the results to the understanding of the structural reliability of nitride fuel pellets is discussed. Work supported under DOE/NE Agreement # DE-FC07-05ID14654.

9:30 AM
Development of a Ceramic-Lined Crucible for the Separation of Salt from Uranium: *Brian Westphal*[1]; Ken Marsden[1]; JC Price[1]; [1]Idaho National Laboratory

As part of the spent fuel treatment program at the Idaho National Laboratory, alternate crucible materials are being developed for the processing of uranium and salt. The separation of salt (LiCl/KCl based) from uranium is performed in an inductively-heated furnace capable of distillation under vacuum conditions. Historically, salt and uranium have been processed in graphite crucibles coated with a zirconia mold wash. Although the coated crucibles have performed adequately considering the reactive nature of salt and uranium at high temperature, the operations required for multiple use of the crucibles are quite labor intensive. Thus, an alternate ceramic-lined crucible has been developed to eliminate the interim operations. Two ceramic-lined crucibles have been tested using irradiated materials to verify their compatibility and determine an ultimate life-cycle. Results from the testing program will be presented on crucible deterioration and other cumulative effects.

9:50 AM
Microscopic and Spectroscopic Characterization of Aluminosilicate Waste Form with Cs/Sr Loaded Using SEM, TEM and XRD: *Gary Cerefice*[1]; Longzhou Ma[1]; [1]University of Nevada Las Vegas

The goal of this work is the characterization of an aluminosilicate waste form for the storage and ultimate disposal of an isolated cesium and strontium waste stream. The aluminosilicate waste forms with/without Cs/Sr loading were synthesized from bentonite clay at different sintering temperatures to examine the impact of fabrication temperature on waste form. TGA and DTA analysis for the synthesized waste forms were conducted, identifying the temperatures where interstitial water is driven from the waste former matrix. Microscopic and spectroscopic characterization of the synthesized waste forms was conducted using SEM, TEM and XRD. The SEM analysis results show the sponge-like morphology of the synthesized materials. Further analysis by TEM, HRTEM and XRD indicates that the waste stream components are actually segregated into discrete phases, and that these discrete, sub-micron particles are distributed throughout the matrix. EDX examination was also performed to identify the chemical composition of these particels and substrate.

10:10 AM Break

10:20 AM
Quantification of Microstructurally Induced Variability on the Thermo-mechanical Response of Nitride Nuclear Fuels through Finite Element Models: *Manuel Parra Garcia*[1]; Pedro Peralta[1]; Kirk Wheeler[1]; Ken McClellan[2]; [1]Arizona State University; [2]Los Alamos National Laboratory

A two-dimensional (2D) finite element model of a cylindrical fuel pellet has been formulated to investigate the variability of the thermo-mechanical response due to microstructure heterogeneity within a Representative Volume Element (RVE). Microstructural information was obtained from sintered ZrN as a surrogate for PuN, processed under conditions similar to those used in actinide bearing fuels. The 2-D RVE obtained from microstructural characterization, which includes pore and grain geometry as well as grain orientation, is surrounded by "effective material" and located at different positions in the model to evaluate variations in stresses strains, and temperature fields within the RVE. The models account for different boundary conditions, as well as creep, thermal expansion and radiation swelling. This effort is directed towards the formulation of a framework that can be translated into characterization and modeling of actual fuels to improve simulations of fuel performance. Work supported under DOE/NE Agreement # DE-FC07-05ID14654.

10:40 AM
Miniaturized Specimen Testing of Monolithic Fuels and Structural Materials: *Ramprashad Prabhakaran*[1]; James Cole[1]; Douglas Burkes[1]; Jian Gan[1]; Indrajit Charit[2]; [1]Idaho National Laboratory; [2]University of Idaho

Efforts are ongoing to develop new nuclear fuels to enable research and test reactors to use low-enriched uranium fuels instead of high-enriched uranium fuels, without significant loss in performance. Hence, a new monolithic fuel type, where the fuel region consists of a single U-Mo (Uranium-Molybdenum) foil encased inside aluminum cladding, is being developed. Understanding fuel foil mechanical properties and fuel/cladding bond strength in monolithic plates is of paramount importance. Efforts are also underway to investigate advanced structural/cladding materials for the next generation reactors. The irradiated materials currently being studied include MA 754, MA 957, 800H and T122. Hence, in this study, the mechanical properties of monolithic fuel foils and irradiated structural materials were evaluated using small-scale specimen testing techniques such as shear punch, micro-hardness and sub-size tensile testing. Optical microscopy, SEM and TEM were used to study the microstructural characteristics.

Materials in Clean Power Systems IV: Clean Coal-, Hydrogen Based-Technologies, and Fuel Cells: Solid Oxide Fuel Cell Materials, Session II: Interconnects

Sponsored by: The Minerals, Metals and Materials Society, ASM International, TMS Electronic, Magnetic, and Photonic Materials Division, TMS/ASM: Corrosion and Environmental Effects Committee, TMS: Energy Harvesting and Storage Committee
Program Organizers: K. Scott Weil, Pacific Northwest National Laboratory; Michael Brady, Oak Ridge National Laboratory; Ayyakkannu Manivannan, US DOE; Z. Gary Yang, Pacific Northwest National Laboratory; Xingbo Liu, West Virginia University; Zi-Kui Liu, Pennsylvania State Univ

Thursday AM — Room: 3005
February 19, 2009 — Location: Moscone West Convention Center

Session Chairs: Gordon Xia, Pacific Northwest National Laboratory; Ayyakkannu Manivannan, US DOE

8:30 AM Introductory Comments

8:35 AM Invited
Ferritic Steel Interconnects for SOFC Systems: Corrosion and Protection: *Paul Gannon*[1]; Max Deibert[1]; Preston White[1]; Richard Smith[1]; [1]Montana State University

Ferritic stainless steels with and without protective coatings have been developed for solid oxide fuel cell (SOFC) interconnect applications (~800°C). The effects of alloy and coating composition and morphology on SOFC interconnect-relevant performance are reviewed. Minor differences in alloy composition are associated with significant differences in surface corrosion behavior. Differences in coating composition and mode of deposition can also significantly influence protection capacity. Observations and interpretations are discussed in context of developing inexpensive and durable SOFC interconnects.

9:10 AM
Thermal and Electrical Stability of New Aluminizing Process in Planar SOFC Stacks: *Jung Pyung Choi*[1]; K. Scott Weil[1]; [1]Pacific Northwest National Laboratory

The list of candidate high-temperature alloys considered applicable in SOFCs includes those that form a stable, protective chromium-, silicon-, or aluminum oxide scale in-situ during use. However both chromia and silica volatility occur at high temperature (>600°C), particularly in water vapor bearing environments. Additionally these species preferentially adsorb at the cathode/electrolyte interfaces of cells and cause continual degradation in the overall power output of the fuel cell system. This presentation will discuss the development of a new process (reactive air aluminizing) that results in a stable, Cr-free oxide coating. The process is a powder-based technique that employs diffusion between stainless steel and aluminum in an air environment. The basic concept will be outlined and results (including Cr volatility, thermal expansion, and ASR testing) obtained on aluminized Crofer 22APU will be described. In addition, a mechanism of how the process provides oxidation and Cr volatility protection will be discussed.

9:30 AM
High Temperature Studies on the Ag-CuO Air Braze Filler Metal System: *Jens Darsell*[1]; K. Scott Weil[1]; [1]Pacific Northwest National Laboratory

A series of high-temperature studies have been conducted on the Ag-CuO system to understand its viability in creating long-lasting, oxidation ceramic-ceramic and ceramic-metal joints for various electrochemical applications (e.g. solid oxide fuel cells, gas separation devices, and high-temperature sensors). These studies include: an investigation of phase equilibria in the Ag–CuO system using a combination of thermal, microstructural and compositional analyses, high-temperature wetting experiments, and in-situ observations of wetting transitions between select Ag-CuO compositions and various substrates. Taken as

a whole, the results from each series of experiments exhibit an interesting set of interrelated relationships. We will present and discuss these findings specifically as they pertain to investigating potential compositional modifications to the Ag-CuO system and more broadly as possible tools for exploring high-temperature wetting phenomena in other liquid-solid phase material systems.

9:50 AM Break

9:55 AM Invited
Exploration of Alloy 441 Chemistry for SOFC Interconnect Application: *Paul Jablonski*[1]; Christopher Cowen[1]; [1]NETL

Alloy 441ss is being considered for application as an SOFC interconnect. There are several advantages to this selection: First and foremost this production alloy is low cost and readily available. Second, the coefficient of thermal expansion (CTE) is compatible with ceramic components of the fuel cell. Third, this alloy forms Laves phase at SOFC operating temperatures. Laves phase has been shown to preferentially consume the Si in the alloy thus avoiding the formation of electrically resistive Si rich oxide subscales which have been shown to be detrimental to SOFC operation. In this paper we will explore the alloy 441ss metallurgy through the use of computational thermodynamics and discuss them with regards to Laves phase formation under SOFC operating conditions. We find that special care must be employed in alloy specification to insure that Laves phase is available to remove Si from the matrix and thus insure useful SOFC operation.

10:30 AM
Comparison of MnCo Coated SS430 and T441 for SOFC Interconnect: *Junwei Wu*[1]; Christopher Johnson[2]; Xingbo Liu[1]; Randall Gemmen[2]; Yinglu Jiang[1]; [1]West Virginia University; [2]National Energy Technology Lab

Ferritic stainless steel SUS430 and T441 are one of the most promising candidate for SOFC interconnect. With the addition of Nb, Ti in T441, the formation of continuous silica sub-layer can be avoided, which is attributed to Nb and Si rich secondary phase formation to stabilize silicon. However, it is not clear how the secondary phase affect the diffusion of substrate elements, Mn, Cr and Fe. Electrodeposition of MnCo alloys with the following oxidation has been proved to be effective for interconnects coating. In this work, MnCo coated SUS 430 and T441 by pulse plating has been oxidized at 800°C for different times. Then surface and cross-section SEM/EDX test are used to study the elements diffusion and secondary phase effect. Furthermore, uncoated and MnCo coated SUS430 and T441 interconnect on button cell test has been conducted to compare the cell performance degradation.

10:50 AM
Mixed Conductive Coatings on Metallic Interconnects in SOFCs: *Zhenguo "Gary" Yang*[1]; Gordon Xia[1]; Josh Templeton[1]; Zimin Nie[1]; L. Shari Li[1]; Chong-Min Wang[1]; Jeff Stevenson[1]; Prabhakar Singh[1]; [1]Pacific Northwest National Laboratory

In intermediate-temperature planar SOFC stacks, stainless steels are used as promising candidates for construction of interconnects, that electrically connect neighboring cells and hermetically separate fuel at the anode-side and air at the cathode-side. For long-term operation at temperatures that are allowed by current cell materials and technologies however, further improvement is required in their surface stability and the electrical resistance arising from the oxide scale growth. For this purpose, the ferritic stainless steels are surface-modified via application of a conductive oxides protection layer. In the past couple of years, PNNL has been conducting this investigation and developing the protection layers and fabrication approaches. This paper will give an update on our efforts in this area.

11:10 AM
Development of MnCoO Coating with New Aluminizing Process for Planar SOFC Stacks: *Jung Pyung Choi*[1]; K. Scott Weil[1]; Yeong-Shyung Chou[1]; Jeffry W. Stevenson[1]; Zhenguo "Gary" Yang[1]; Prabhakar Singh[1]; [1]Pacific Northwest National Lab

Low-cost, chromia-forming steels find widespread use in SOFCs at operating temperatures below 800°C, because of their low thermal expansion mismatch and low cost. However volatile Cr-containing species originating from this scale poison the cathode material in the cells and subsequently cause power degradation in the devices. To prevent this, a conductive manganese cobaltite coating has been developed. However this coating is not necessarily compatible with forming hermetic seals between the interconnect or window frame component and ceramic cell. Thus, a new aluminizing process has been developed for the sealing regions in these parts, as well as for other metallic stack and balance-of-plant components. This paper will present the basic processes used in each coating technique and discuss some of the compatibility issues that arise when integrating both coatings into the same component.

11:30 AM
Development of Electrical Contacts between Cathodes and Metallic Interconnects in SOFCs: *Gordon Xia*[1]; Zhenguo "Gary" Yang[1]; Josh Templeton[1]; Jeff Stevenson[1]; [1]Pacific Northwest National Lab

In SOFCs, electrical contacts or contact layers are applied between electrodes (anode or cathode) and interconnects to promote electrical contact and facilitate stack assembling. Particularly the electrical contact at the cathode-side is essential to offer a low resistant electron transport bridge that connects a metallic interconnect and perovskite cathode. One promising group of materials for the contact layers are conductive oxides that nevertheless often demonstrate an inferior sintering activity for this particular applications. PNNL has searched suitable materials and developed approaches to fabricate the contact layers with emphasis on improving the materials sintering activity. This paper will present details of this work.

Nanocomposite Materials: Nanocomposite Processing

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS Electronic, Magnetic, and Photonic Materials Division, TMS/ASM: Composite Materials Committee, TMS: Materials Characterization Committee, TMS: Nanomaterials Committee
Program Organizers: Jonathan Spowart, US Air Force; Judy Schneider, Mississippi State University; Bhaskar Majumdar, New Mexico Tech; Benji Maruyama, Air Force Research Laboratory

Thursday AM — Room: 3020
February 19, 2009 — Location: Moscone West Convention Center

Session Chairs: Jonathan Spowart, US Air Force; Francisco Robles Hernandez, University of Houston

8:30 AM Introductory Comments

8:35 AM Invited
Consolidation of Bulk Nanocomposites Using Current Activated Densification: *Javier Garay*[1]; [1]University of California, Riverside

Nanocrystalline ceramics display significantly different properties than their microcrystalline counterparts, yet they have been difficult to produce in bulk sizes. The versatile material processing technique of current-activated pressure assisted densification has proven effective in densifying nano-ceramic powders into bulk nanomaterials. Results on large-sized, fully dense oxide ceramics with crystal sizes much less that 100nm will be presented. In particular we will focus on our recently developed processing technique that leverages metastability to partially transform phases producing nanocomposites with very clean epitaxial-like interfaces. These materials display unique functional and structural properties. Properties discussed include improved visible light transmittance and novel magnetic properties.

9:00 AM
Development of Nanostructured Polyurethanes Materials for Anticorrosive Coatings: *Ariosvaldo Sobrinho*[1]; Luiz Pontes[2]; Rejane Dantas[2]; André Rodrigues[1]; Edjânio Araujo[2]; [1]CCT / Materials; [2]UFPB

Nanocomposites based on Polyurethane/organophilic clay solutions were obtained using methyl ethyl ketone (MEK) like organic solvent. Various organo-modified clays were prepared in solution and their morphology, adhesive force, shock-resistant toughness, densification of lacquer surface and anti-corrosion were evaluated in coating anticorrosive applications. For better performance of solvent-based polyurethane for anticorrosive coatings applications, they were modified either by varying polyurethane microstructures or by dispersing inorganic fillers, especially by incorporating nanosized layered silicates within the polyurethane continuous matrix. The main objectives of this work were the synthesis of solvent-based polyurethane using organophilic clay and their study by TGA, morphology, adhesive force, shock-resistant toughness, densification and anti-corrosion properties. The most significant feature of this investigation

is the improve of adhesive force, shock-resistance toughness and anti-corrosion of various chemical media so that it is possible to resolve various problems in materials applied to petroleum applications industry.

9:20 AM
Dispersing of Nano-Particles in Molten Aluminum Using High-Intensity Ultrasonic Vibrations: Clause Xu[1]; Lu Shao[1]; *Qingyou Han*[2]; [1]Hans Tech; [2]Purdue University

The most inexpensive method for processing particle reinforced aluminum matrix composites involves the use of a stirrer for dispersing particles in molten metal. The method is successful in making composites containing particles larger than a few microns but is difficult in dispersing particles in the nano-size range (<100 nm). This article discusses an enabling technology for dispersing nanoparticles in molten metal using high-intensity ultrasonic processing technology. The use of high-intensity ultrasonic vibration breaks up the nanoparticle clusters and disperses the individual nanoparticles into the melt. The resultant nanocomposites are of superior mechanical properties especially tensile and creep resistance at elevated temperature. Issues associated with the dispersing of nano-particles are addressed.

9:40 AM
Influence of Dispersed Carbon Nano-Fibers/Carbon Nano-Tubes in Al Matrix Composite: *Minoru Oda*[1]; Chitoshi Masuda[1]; Fumio Ogawa[1]; Seiji Itabashi[1]; Toshiyuki Nishimura[2]; [1]Waseda University; [2]National Institute for Materials Science

CNT and CNF are cohered by Van der Waals force, and the cohesion of CNT and CNF deteriorates the properties of the composite material such as strength, elastic modulus remarkably. First, the influence of surfactant is examined by comparing dispersd CNT, CNF and without dispersed ones. The dispersion state is observed by TEM and SEM. Secondly, mechanical properties of composites made by using surfactant are also examined and compared with those ones made without using surfactant. CNT and CNF are dispersed by using ultrasonic shaker and dried in homoiothermal chamber. Next, dispersed ones are mixed with Al powder (30μm) in ball mill for 3 hours by rotating at 200 rpm. After that, mixed powders are sintered by SPS. The pressure of SPS is held at 200MPa and the hold time is 5 minutes. Mechanical properties of composites made using above two methods will be measured.

10:00 AM
Influence of Solvent on Dispersion State of the Reinforcement in Magnesium Matrix Composites: *Seiji Itabashi*[1]; Chitoshi Masuda[1]; Fumio Ogawa[1]; Minoru Oda[1]; Toshiyuki Nishimura[2]; [1]Waseda University; [2]National Institute for Materials Science

Carbon nanotubes (CNT) and carbon nanofibers (CNF) have superior characteristic, such as high strength, high Young's modulus. However, CNT and CNF are cohered by Van der Waals force and the cohesion of CNT and CNF deteriorates the properties of the composite material such as strength remarkably. Primarily, influence of solvent on composite material is examined by dispersing CNT and CNF using surfactant. For comparison, it is examined without solvent. Secondly, mechanical properties of composites produced using above solvent are also examined and compared with that of one produced without solvent. CNT and CNF are dispersed in solvents using ultrasonic shaker and the solvent is dried in homoiothermal chamber. Next, the carbon powder is mixed with magnesium powder (180μm) in the ball mill. After mechanical alloying, mixed powder is sintered using SPS. Mechanical properties of composites produced using two methods, mechanical and physical properties will be measured.

10:20 AM Break

10:35 AM
Production of Metal Matrix Composites with CFullerene and CGraphite Reinforcements: *Francisco Robles Hernandez*[1]; Hector Calderon Benavides[2]; [1]University of Houston; [2]Instituto Politécnico Nacional

In the present work are reported the results of the production of nanostructured Al and Fe matrix composites with reinforcements of CGraphite or CFullerene (C60 + C70 + CSoot) sintered by means of Spark Plasma Sintering (SPS) and characterized by means of XRD, SEM and TEM. CFullerene withstands longer mechanical milling or alloying showing batter control agent characteristics when compared to CGraphite. The SPS method preserves the nanometric nature of the composites and the full transformation of CFullerene into Al4C3. For the Fe-CFullerene composite the CFullerene is not affected by mechanical alloying SPS processes; an apparent transformation of the CSoot into CFullerene and Orthogonal CFullerene are identified; followed by a transformation to diamond by thermomechanical means. The sintered, by SPS, products showed an increase in hardness for in the final composites being the composites with CFullerene the ones with higher hardness.

10:55 AM
Ultrafine-Grained Aluminum Alloy and Boron Carbide Composite Extrusions: *Rustin Vogt*[1]; Zhihui Zhang[1]; Troy Topping[1]; Enrique Lavernia[1]; Julie Schoenung[1]; [1]University of California, Davis

Ultrafine-grained aluminum alloys have shown significant increases in strength with addition of ceramic particulate reinforcement. In the present study, boron carbide (B4C) particulate (1-7 micron) was cryomilled together with Al 5083 to form a nanocrystalline composite powder (i.e. grain size ~27 nm). The nanocomposite powder was blended with un-milled Al 5083 powder and processed by different consolidation routes to form ultra-fine grained bulk composites. The processing effects of hot isostatic and cold isostatic pressing as well as dynamic and quasi-static extrusion rate have been investigated on basis of the resulting microstructure, mechanical properties and fracture behavior of the final extrusions.

11:15 AM
Thermal Stability of a Lamellar Nanocomposite Al/AlMg3 Prepared by Accumulative Roll Bonding: *Margarita Slamova*[1]; Peter Slama[2]; Petr Homola[1]; Jaromir Uhlir[1]; Miroslav Cieslar[3]; [1]COMTES FHT, Ltd.; [2]VUK Panenske Brezany, Ltd.; [3]Charles University in Prague

High strength ultrafine-grained (UFG) materials can be prepared by accumulative roll bonding (ARB). Their low ductility however represents a grave drawback in many applications. The ductility problem can be resolved in materials with bimodal grain size distributions with good yield strength and fairly large uniform elongation. A lamellar composite with grains of submicrometer size was prepared by ARB from Al and AlMg3 sheets. The thermal stability of the UFG structure was investigated in the temperature range 150-350°C. The grain size was evaluated by various microscopy methods, including EBSD. AlMg3 composite layers remained unrecrystallized up to 250°C, whereas the Al layers started recrystallizing at much lower temperature. Bimodal grain size distributions shifted to smaller sizes with increasing ARB cycles were observed in the annealed materials. The evolution of strength with number of cycles and temperature was monitored by hardness and tensile tests. The composite was compared with mono-material ARB sheets.

11:35 AM
Mg Matrix Nano Composites: *Ari Erman*[1]; Joanna Groza[1]; Xiaochun Li[2]; Guoping Cao[2]; Hong-seok Choi[2]; Prashant Soni[3]; [1]University of California, Davis; [2]University of Wisconsin-Madison; [3]Indian Institute of Technology Bombay

Mg matrix nanocomposites, reinforced with SiC nanoparticles, have been cast by ultrasonic cavitation based dispersion methods. Microstructural studies of as cast specimens are done to characterize the grain and dislocation structure and SiC particle size and distribution. We plan to carry out low cycle fatigue experiments of Mg-SiC nano composites.

Near-Net Shape Titanium Components: Powder Metallurgy II

Sponsored by: The Minerals, Metals and Materials Society, TMS: Titanium Committee
Program Organizers: Rodney Boyer, Boeing Company; James Cotton, Boeing Co

Thursday AM — Room: 2010
February 19, 2009 — Location: Moscone West Convention Center

Session Chair: M. Ashraf Imam, Naval Research Laboratory

8:30 AM
Cost-Effective Titanium Alloy Powder Production and Consolidation for Near-Net Shaped Component Manufacturing: *Deliang Zhang*[1]; Stiliana Raynova[1]; Vijay Nadakuduru[1]; Brian Gabbitas[1]; Barry Robinson[2]; [1]University of Waikato; [2]South Auckland Forging Engineering Ltd (SAFE)

This paper will first briefly introduce a newly developed cost-effective titanium alloy powder production process, the TiPro process, which utilises

relatively low cost TiO2 and Al powders and other reactants as raw materials, and involves solid-liquid separation and powder purification. Findings from a study on the effects of thermomechanical consolidation conditions on the defects, microstructure and mechanical properties of the consolidated samples of titanium and Ti-Al based alloys such as Ti-6wt%Al-4wt%V alloy will also be presented and discussed. At this stage of the project, the major aim of the research is to develop a novel thermomechanical powder consolidation process that can be used to produce semi-finished titanium alloy products such as forged blocks and rolled plates cost effectively. The longer term goals of the research on powder consolidation also include development of cost-effective powder consolidation processes for manufacturing titanium alloy near-net shaped components for various applications.

8:50 AM

Development and Manufacturing of the Near Net Shape Parts from Ti Alloys with the Reduced "Buy to Fly" Using PM HIP Route Based on the Process Modeling: *Victor Samarov*[1]; C. Barre[1]; D. Poor[2]; [1]Synertech PM; [2]Kittyhawk Products Inc

The general task of HIP modeling is in designing the initial shape of the HIP tooling providing the final "net" or "near net shape" part after HIP consolidation of powder. The core of modeling is the description of the mutual deformation of the compressible (powder) and non-compressible (HIP tooling) materials. The paper presents the results of development efforts providing adequate description of the HIP deformation for parts from Ti alloys of the different geometrical complexity and physical non-uniformity mainly used for the aerospace applications.Such process modeling associated with the novel design of the HIP tooling enables to manufacture "selectively net shape" and "near net complex shape" parts for different static and rotating applications requiring no or minimal machining of the critical (and difficult to machine) surfaces and cutting down substantially the buy-to fly ratio for various aerospace components.

9:10 AM

Fabrication of Titanium Shrouded Impellers for Rocket Engine Liquid Hydrogen Pumps: *Cliff Bampton*[1]; Victor Samarov[2]; John Wooten[3]; [1]Pratt & Whitney Rocketdyne; [2]Synertech Inc.; [3]CalRAM Inc.

A case study is presented for competing methods of fabricating titanium alloy shrouded impellers. These are critical components in liquid hydrogen fueled rocket engines. The shrouded impeller design, optimized for pump performance, makes conventional fabrication - machining of die forgings - difficult and expensive with long cycle times. Three alternate net and near-net shaping processes are compared: Investment casting; Powder metal hot isostatic pressing; Powder metal additive layered build by electron beam melting. Attributes and limitations of each process are demonstrated and discussed.

9:30 AM

New Possibilities of Enhancing Mechanical Properties and Microstructure for Conventional Ti Alloys via the PM HIP near Net Shape Route: *I. Polkin*[1]; Victor Samarov[2]; [1]VILS; [2]Synertech PM

It is acknowledged today that Ti parts obtained via PM HIP route have better uniformity and homogeneity compared to cast and wrought material, however the latter still keeps the advantages in mechanical properties. The paper presents the results of the development work on PM HIP of near net shape parts from Ti alloys with the enhanced micro-structure and mechanical properties. These new advantages are gained due to the exceptionally fine and uniform micro-structure that can be achieved as a result of the special processing including encapsulation and HIP. The results obtained for the complex shape parts from the conventional grades of Ti alloys are compared to the micro-structure and mechanical properties of the parts made via conventional forging of billets. It is demonstrated that the mechanical properties of PM HIPed material are at the same level or even higher that those of the cast and wrought material with substantial reduction of the processing steps to produce them to the desired shape.

9:50 AM Break

10:10 AM

Study of Sintering Behavior of Ultrafine Titanium Powders: *Hongtao Wang*[1]; Zhigang Fang[1]; [1]University of Utah

The near net shape (NNS) capability of powder metallurgy (PM) techniques can dramatically reduce the cost of titanium components. It is well known that sintering behaviour of a metal powder is related to its particle size, and the sintering can be significantly enhanced via the refinement of powder size. In this investigation, the size-dependent sintering behaviour of titanium powders has been studied by sintering of different-sized titanium powders (coarse and ultrafine) using a dilatometer. The ultrafine powders were produced via high-energy mechanical milling. The results show that the sintering temperature of ultrafine titanium powder decreases remarkably compared to that of the sintering of conventional coarse powder, and as a result, better sintering densification is achieved by using ultrafine titanium powder. Dilatometric data are used to study the difference of sintering process and kinetics between coarse Ti powder and ultrafine Ti powder, and the mechanisms of densification will also be discussed.

10:30 AM

Low Temperature Compaction of Titanium Alloy Powder by Equal Channel Angular Extrusion with Back Pressure: *Rimma Lapovok*[1]; Dacian Tomus[1]; [1]Monash University

It is shown that the use of Equal Channel Angular Extrusion (ECAE) with applied back pressure for compaction of powder allows significantly decrease the temperatures of consolidation compare to those used in conventional practice. The possibility to lower the processing temperature would give a cost-effective method to produce a cheaper product as well as minimise the contamination of powder and compact with gaseous constituents known to be harmful to resultant properties. The novelty of the approach arises from the notion that severe shear deformation triggers several physical mechanisms contributing to improved compaction. The compacts produced from CP-Ti at temperatures in the range from room temperature to 300°C by ECAE with back pressure have a relative density above 99.5%. Efficient consolidation of pre-alloyed (PA) Ti-6Al-4V (HDH) powder at temperatures of 400°C and below, achieving relative densities of 98.3-98.6% and green strengths up to 750 MPa has been performed.

10:50 AM

Stress-Corrosion Cracking and Fatigue Crack Growth of Consolidated Powder of Ti-6Al-4V: Peter Pao[1]; *M. Ashraf Imam*[1]; Robert Bayles[1]; Jerry Feng[1]; [1]Naval Research Laboratory

Ti-6Al-4V plates, consolidated from powders, manufactured from Armstrong-process and hydride-process were studied. The Armstrong-process allows direct production of titanium powder in a single step in-situ reaction whereas the hydride-process uses the hydrogenation of the ore. Both processes result into considerable savings when compared to converting sponge to powder. The yield strengths of these plates are about 920 MPa. The oxygen content from hydride-process is higher compared to the Armstrong-process(0.3 vs. 0.2 wt%). Preliminary fatigue crack growth study indicates that, in the as-received condition, the threshold stress intensities of Armstrong-process and hydride-process approaches to that of the conventional cast-ingot of Ti-6Al-4V. The stage II fatigue crack growth rates of hydride-process are substantially higher than that of the Armstrong-process and the conventional cast-ingot-cast. The mechanism of the fatigue crack growth rates difference, fracture toughness, and stress-corrosion cracking resistance of Ti-6Al-4V will be discussed.

11:10 AM

Use of Rapid Solidification to Affect Ultra-Refined Microstructures in Near-Net Shape Materials: *Peter Collins*[1]; Jonathan Orsborn[1]; Hamish Fraser[1]; [1]Ohio State University

Directed laser deposition techniques, such as laser engineered net shaping (LENS™), will often exhibit solidification and cooling rates approaching rapid solidification ($\Delta T \sim 1000°C/sec$). It is possible to exploit the resulting ultra-refined microstructures to control properties. Using both conventional processing and LENS™ processing, ultrafine distributions of alpha-precipitates will be affected in Ti-6Al-4V, Ti-6-2222, and model alloy based on the Ti-Al-Mo system. The mechanical properties of these materials will be probed and correlated with microstructural length scale.

Neutron and X-Ray Studies of Advanced Materials: Neutron Diffraction and Modeling of Materials Behavior

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Titanium Committee
Program Organizers: Rozaliya Barabash, Oak Ridge National Laboratory; Yandong Wang, Northeastern University; Peter Liaw, The University of Tennessee; Jaimie Tiley, US Air Force

Thursday AM Room: 3016
February 19, 2009 Location: Moscone West Convention Center

Session Chairs: Judy Pang, Oak Ridge National Laboratory; Jaimie Tiley, US Air Force

8:30 AM Keynote
In-Situ Neutron Scattering Studies of Multi-Ferroics under Stress, Temperature and Magnetic Fields: *Donald Brown*[1]; [1]Los Alamos National Laboratory

Multi-ferroic materials, such as shape memory alloys, ferro-electrics, and ferromagnetic shape memory alloys have been studied heavily recently. Despite being driven by distinct stimuli, such as stress or magnetic field, the underlying physics of multi-ferroic materials is similar. Relatively large and recoverable dimensional changes are achieved by either large scale crystal reorientation (variant selection) or phase transformation. Time-of-Flight (TOF) neutron diffraction is uniquely suited to study multi-ferroics because neutrons penetrate into the bulk and the TOF technique allows us to record the entire diffraction pattern (0.5-4Å) simultaneously. This talk will highlight the technique and our efforts to study various multi-ferroic materials including shape memory alloys, such as U6Nb and NiTi, magnetic shape memory alloys, such as Ni2MnGa, and ferro-electrics under conditions of monotonic and cyclic loading, elevated temperature, and applied magnetic field on the SMARTS diffractometer at the Lujan Center.

9:00 AM Invited
Advances in Modeling Internal Strain Evolution of Aggregates: *Carlos Tome*[1]; Bjorn Clausen[1]; John Neil[2]; Sebastien Merkel[3]; [1]Los Alamos National Laboratory; [2]University of Virginia; [3]University des Sciences et Technologies de Lille

Polycrystal models are used for simulating and interpreting in-situ internal strain measurements done with neutron and X-ray diffraction. Our Elasto-Plastic Self-Consistent (EPSC) model has proven effective not only in providing interpretation of experimental results, but also insight into the crystallographic mechanisms responsible for plasticity. In this presentation we discuss new capabilities of our EPSC approach and how they impact our understanding of polycrystal plasticity. First, accounting for texture evolution allows us to address the large strain regime; results for Cu and stainless steel will be discussed. A second modeling advance allows us to account for twin reorientation and for the stress relaxation associated with it; experimental and modeling results will be presented for Mg AZ31. Finally, the interpretation of results for Co (hcp) tested to 50 GPa pressure, reveals the role played by plasticity in controlling stress build-up under high pressure.

9:20 AM
Characterization of Gamma and Gamma Prime Phases in Nickel Base Superalloys Using Neutron Diffraction and XRD Techniques: *Jaimie Tiley*[1]; R. Srinivasan[2]; R. Banerjee[3]; Hamish Fraser[2]; B. Viswanathan[3]; [1]US Air Force; [2]Ohio State University; [3]University of North Texas

Gamma and Gamma Prime precipitates in a nickel base superalloy were characterized using advanced neutron diffraction and x-ray diffraction techniques. Specifically, volume fraction, chemical composition, residual stresses, and lattice parameters were determined and used in Rietveld refinements to determine lattice site occupancies of alloying elements. Rene88 material was treated to three different cooling rates and then aged up to 200 hours to provide different microstructures. Material parameters were measured as a function of cooling rates and aging times. In addition, samples were heated in situ to obtain neutron diffraction data at temperatures up to 600°C. Results link microstructures to heat treatment conditions and compare different characterization techniques.

9:40 AM
Evolution of Crystallographic Texture of TRIP Steel after Multi-Axial Deformation: *Adam Creuziger*[1]; Thomas Gnaeupel-Herold[1]; Timothy Foecke[1]; Mark Iadicola[1]; Stephen Banovic[1]; [1]NIST

TRIP (Transformation Induced Plasticity) steel is a high strength, high ductility steel alloy being investigated as a replacement for conventional steel used in outer body panels and internal structure of automobiles. In this study, as received TRIP 780 steel sheets were deformed under a variety of in plane multi-axial conditions and the elastic and plastic strains were measured in-situ. After deformation the phase fraction of the deformed material and crystallographic texture was determined using neutron and x-ray diffraction. The results of the samples deformed under multi-axial loads will be compared to uniaxial tension tests and the experimentally determined effect of loading path on deformation, phase fraction and texture will be discussed.

9:55 AM
In-situ Neutron Diffraction of the Anomalous Ductility of CoTi and CoZr B2 Intermetallics: *James Wollmershauser*[1]; C. Neil[1]; Sean Agnew[1]; [1]University of Virginia

Fully-ordered B2 compounds, CoTi and CoZr, are examined by in-situ neutron diffraction during compression testing at room temperature. Previous studies have shown that both alloys can accommodate appreciable elongation, up to 20% in CoZr, while TEM studies have shown only dislocations with <100> Burgers vectors, which suggests that there are insufficient independent slip systems to accommodate arbitrary strains at the grain level. Such anomalous ductility is similar to that reported of B2 compounds composed of rare earth elements in combination with late transition elements, such as AgY and CuDy. Modeling of the measured internal strain evolutions using the elastoplastic self-consistent (EPSC) polycrystal plasticity code is used to explore the mechanisms of plastic deformation and the results are compared to an earlier neutron diffraction study of a rare earth-containing comound, AgCe, and conventional intermetallics, NiAl and CuZn.

10:05 AM
Effects of Overload and Underload on the Residual Stress, Crack-Opening Load, and the Crack-Growth Behavior: Soo Yeol Lee[1]; *Peter Liaw*[1]; Hahn Choo[1]; Ronald Rogge[2]; Michael Gharghouri[2]; [1]University of Tennessee; [2]Chalk River Laboratories

Various fatigue-loading conditions (i.e., fatigued, tensile overloaded, compressive underloaded, tensile overloaded-compressive underloaded, and compressive underloaded-tensile overloaded) were introduced to study the crack-growth retardation/acceleration mechanisms during fatigue crack growth. First, the spatially-resolved neutron-strain mapping was performed to measure three principal residual-strain components developed near a crack tip under the various loading conditions, and then residual-stress distributions were calculated as a function of the distance from the crack tip. Second, the electric-potential technique was employed to determine the crack-opening load associated with the crack-tip driving force at different crack-growth stages. Finally, the relationship among the residual stress, crack-opening load, and the crack-growth rate is investigated, and the mechanisms concerning the overload/underload effects are suggested.

10:15 AM
Formation of Deformation Textures in F.C.C. Materials Studied by In-Situ Neutron Diffraction and Self-Consistent Model: *Nan Jia*[1]; Yandong Wang[1]; Ru Peng[2]; X. Zhao[1]; [1]Northeastern University; [2]Linköping University

Polycrystalline f.c.c. materials usually deform in a variety of slip, twinning and shear banding modes and exhibit marked plastic anisotropy at the grain level. This causes the evolution of preferred grain orientation distribution (crystallographic texture) that affects again the distribution of heterogeneous stresses within materials. In the current work, in-situ neutron diffraction experiments were employed on f.c.c. metals (copper, aluminium and brass) with different stacking fault energy. The evolution of microstresses in each metal was traced under the stress field.Based on the grain-boundary-mediated activities that were experimentally characterized as the lattice strain distributions of multiple reflections, deformation textures of the different materials were simulated with an Elastic-Plastic Self Consistent (EPSC) model. The featured slip systems and stress/stain states were selected according to the accommodation of misfits

among grains. Such an approach thus provides an unambiguous understanding on the micromechanics of texture development in various f.c.c. materials under external load.

10:30 AM Break

10:40 AM Invited

High-Pressure Studies of Various Materials by Synchrotron-Based X-Ray Diffraction: *Haozhe Liu*[1]; Luhong Wang[1]; [1]Harbin Institute of Technology

The study of polymorphism and polyamorphism in pressure domain will undoubtedly broaden our horizons and perspectives of the states of matter in general, and may have a significant impact on the existing theories about the structure, formation, and evolution of crystal and amorphous materials. The synchrotron x-ray diffraction and diamond anvil cell techniques were used to study these subjects. One typical powder sample, zinc oxide from NIST standards, was selected to study its phase transition mechanism under high pressure and low temperature conditions. Two types of metallic glass were selected to test the pressure induced polyamorphism. The procedure of the pressure-induced amorphous state to crystalline state is another subject in this talk. These will provide new insight on the nature of phase transition, provide new invitation for the electronic theoretical studies for the phase stability, and improve our understanding of the kinetic process of the common pressure induced crystallization.

11:00 AM

Fundamental Studies of Intergranular Strains Evolution in a Zircaloy-4 Alloy with Random Texture: *Elena Garlea*[1]; Bjorn Clausen[2]; Sven Vogel[2]; Judy Pang[3]; Hahn Choo[4]; [1]B&W Y-12 National Security Complex / University of Tennessee; [2]Los Alamos National Laboratory; [3]Oak Ridge National Laboratory; [4]University of Tennessee / Oak Ridge National Laboratory

A Zircaloy-4 alloy with Basketweave - Widmanstätten type microstructure and random texture has been used to study the deformation systems responsible for the polycrystalline plasticity at the grain level. The evolution of internal strains and bulk texture is investigated using neutron diffraction and an elasto-plastic self-consistent (EPSC) modeling scheme. The macroscopic stress-strain behavior and intergranular (hkil-specific) strain development, parallel and perpendicular to the loading direction, were measured in-situ during uniaxial tensile loading. Then, the EPSC model was employed to simulate the experimental results. This modeling scheme accounts for the thermal anisotropy; elastic-plastic properties of the constituent grains; and activation, reorientation, and stress relaxation associated with twinning. The agreement between the experiment and the model will be discussed as well as the critical resolved shear stresses (CRSS) and the hardening coefficients obtained from the model.

11:15 AM

Neutron and X-Ray Diffraction Study of Residual Stress in Creep Deformed Single Crystal Superalloy: *Erdong Wu*[1]; Jinchao Li[1]; Guangai Sun[2]; Bo Chen[2]; V. Ji[3]; V. Klosek[4]; M.H. Mathon[4]; [1]Chinese Academy of Sciences; [2]Institute of Nuclear Physics and Chemistry, CAEP; [3]LEMHE/ICMMO, UMR 8182, Université Paris-Sud 11; [4]Laboratoire Léon Brillouin, CEA Saclay

The redistribution of residual stress state and loss of coherency between the matrix and precipitates are strongly associated with the creep deformation of the single crystal superalloys. However, although estimations have been made, the quantitative measurements on the residual stress are still rare, as the stress measurements on single-crystal are much more complicated than that on poly-crystal sample. In this work, the residual stresses in crept single crystal superalloys were measured by neutron and X-ray diffraction. The evolutions of residual stress and associated lattice distortion and microstrain during the creep deformation were revealed from the analysis of diffraction profiles. A remarkable increase in compressive stress indicating a built-up of residual stress occurred during the low straining stage of creep. The development of the tetragonal lattice distortion for both phases and the greater microstrain along the loading axis associated with stress state change and dislocation were observed.

11:30 AM

Texture and Microstrain Evolution during the Dynamic Recrystallization of Fe: *Tien Tran*[1]; Donald Brown[2]; Benjamin Fell[1]; Joanna Groza[1]; [1]University of California; [2]Los Alamos National Laboratory

Dynamic recrystallization (DRX) during power-law creep is explored as a means to produce large single crystals of alpha-iron by abnormal grain growth (AGG). The current *in situ* neutron diffraction studies focus on the temporal evolution of microstrain and texture during DRX. Typically, recrystallization events during constant-stress creep are inferred from fluctuations in the strain rate. Furthermore, any information obtained from *post mortem* metallography may be contaminated by metadynamic recrystallization. The Spectrometer for Materials Research at Temperature and Stress (SMARTS) at the Los Alamos Neutron Science Center (LANSCE) is a neutron diffractometer designed to study the behavior of bulk materials under extreme loads and temperatures. Creep tests were conducted at various stresses and temperatures to investigate the rate of strain energy accumulation as it relates to grain orientation and the onset of recrystallization. Preferential nucleation/growth leading to texture development was explored as a possible AGG-inducing occurrence.

11:40 AM

Texture Effect and the Role of Deformation Twinning on the Cyclic Deformation of a Rolled Magnesium Alloy, AZ31B: *Liang Wu*[1]; Sean Agnew[2]; Yang Ren[3]; Donald Brown[4]; Bjorn Clausen[4]; Feng Jiang[1]; Peter Liaw[1]; [1]University of Tennessee; [2]University of Virginia; [3]Argonne National Laboratory; [4]Los Alamos National Labortory

Neutron and synchrotron diffraction has been employed to study the cyclic deformation of a rolled magnesium alloy, AZ31B, loaded, respectively, along the rolling direction (RD), transverse direction (TD), and normal direction (ND) at a fully reversed total constant strain amplitude of 3% at room temperature, starting with compression. The initial preferred orientation with the basal poles in most grains aligned along ND favors extensive twinning under in-plane compression or through-thickness tension, and detwinning during the subsequent loading reversals. In-situ neutron diffraction indicates that the twinning and detwinning alternates with the cyclic loading. The texture measurements using synchrotron diffraction suggest the initial texture is completely reversed once detwinning capability is exhausted, concurrent with the disappearance of twin bands. The cyclic deformation behavior is similar for the RD and TD loadings due to the in-plane texture symmetry, while the macroscopic hysteresis under the ND loading is distinct from those under in-plane loadings.

11:50 AM

Continuous Pole Figure Measurement with Neutron Radiation: *Ulf Garbe*[1]; Christian Randau[2]; Christian Hesse[3]; Michael Hofmann[3]; Heinz-Guenter Brokmeier[2]; [1]ANSTO; [2]TU-Clausthal; [3]FRM II

Samples for texture analyses are often coarse grained or samples with sharp texture. Measurements with neutron radiation in a typically 5x5 degree grid will not represent the existing texture. Continuous pole figure measurement instead of step wise technique, will lead to better results with coarse grained material, because every grain is under reflection condition. This technique also decreases beam time for high resolution pole figures, caused on shorter positioning time for the sample orientation. Here we present first results of continuous texture measurements on different type of samples.

12:05 PM

X-Ray Scattering Studies of Orbital Correlations and Quasi-3D Ordered Lattice Modulations in Bilayer Ruthenates with No Long-Range Orbital Order: *Zahirul Islam*[1]; [1]Argonne National Laboratory

X-ray scattering studies of the role of structural correlations across the phase diagram of bilayered ruthenate $(Sr_{1-x}Ca_x)_3Ru_2O_7$ compounds (SCRO) are presented. While the pure Ca end member is an antiferromagnetic insulator, pure Sr compound is an itinerant metamagnet. Bulk measurements reveal disorder-induced unconventional quantum critical behaviors in these materials, in particular, near x=0.3. X-ray scattering studies revealed that robust 2-unit-cell periodic lattice modulations that are characterized by (1/2,0,0) and (0,1/2,0), respectively, even at room temperature, exist at x=0.3 and in the pure Sr compound, but absent in the Ca end member of the series. These modulations are transversely polarized and quasi-3D ordered in that they are fully coherent in the basal plane with c-axis correlations at least one unit cell in extent. These modulations are due to correlated displacements of the O atoms.

Open Source Tools for Materials Research and Engineering: Session I

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS/ASM: Computational Materials Science and Engineering Committee, TMS: Process Technology and Modeling Committee
Program Organizers: Adam Powell, Opennovation; Kim Ferris, Pacific Northwest National Laboratory

Thursday AM Room: 3000
February 19, 2009 Location: Moscone West Convention Center

Session Chairs: Adam Powell, Opennovation; Kim Ferris, Pacific Northwest National Laboratory

8:30 AM Introductory Comments

8:40 AM Invited
NSDL MatDL's MatForge: Open Efforts for Computational Materials Research and Education: *Laura Bartolo*[1]; [1]Kent State University

The Materials Digital Library Pathway (MatDL) is an NSF-supported National Science Digital Library (NSDL) Pathway project to create community-centered, user-tailored access for broad dissemination in the materials community. MatDL is a consortium of organizations including: Kent State University, MIT, National Institute of Standards and Technology, University of Michigan, Purdue University, and Iowa State University. MatDL's MatForge (http://matforge.org), is a Subversion/TRAC workspace for open source development of modeling and simulation codes, serving as a branded, trusted, non-commercial, and neutral site. It hosts mature research code projects, including: FiPy administered by MSEL/NIST code developers and newly launched projects such as OpenThermo, endorsed by the TMS Committee on Integrated Computational Materials Engineering (ICME). As a centralized site with integrated services for developers of team-based materials code projects, MatForge contributes to awareness and use of codes in research and teaching to facilitate development of next generation users in academe and industry.

9:05 AM Invited
The Development of a Public Repository of Interatomic Potentials for Atomistic Simulations: *Chandler Becker*[1]; [1]National Institute of Standards and Technology

With the increasing demand and use of atomistic simulation techniques in materials research and design, the need for a repository of interatomic potentials and the means to compare them becomes ever more important. This is especially true given the sometimes widely different properties calculated using interatomic potentials that are nominally for the same element or alloy. Here we will focus on the development of a public repository to provide a source for vetted interatomic potentials, as well as reference experimental and ab-initio data for comparison. The development of standard evaluation methods (including thermodynamic, kinetic, and mechanical properties) and distribution methods will also be addressed.

9:30 AM
Cyberinfrastructure for Integrated Computational Material Engineering: *Tomasz Haupt*[1]; [1]Mississippi State University

ICME is an approach to design products and materials that comprise them by linking material models at multiple length scales. The complexity of the new generation of simulation codes demands the employment of high-performance computing platforms. Currently, it is a very tedious and error-prone manual effort by the designer to submit, monitor and coordinate hundreds of jobs in heterogeneous distributed environments which requires the designer to learn the arcana of ever-changing IT technologies such as operating systems, batch systems, storage systems, networking, and security. This presentation demonstrates the use of the modern information infrastructure based on Service Oriented Architecture (SOA), Web Services and Grid computing streamlining of the process of gathering experimental results, and deriving the material properties for a particular material model and employing the material model in finite element analysis in the process of building validated metamodels and design optimizations.

9:55 AM Break

10:15 AM Invited
An Integrated Open Source Stack for Thermodynamics and Phase Field Simulations: *Adam Powell*[1]; [1]Opennovation

A public repository of packages for Ubuntu Linux at www.opennovation.org/ubuntu provides several open source engineering software packages for that operating system. This talk will focus on the subset of packages comprising a software stack for integrated computational materials engineering (ICME) calculations. This stack consists of four tools: abinit for DFT energy calculations; ATAT for automating DFT, cluster expansion and Monte Carlo software for calculating the free energy functions of low-energy phases in a system; Ternary for calculating ternary phase diagrams from such free energy functions; and a finite element phase field code for microstructure prediction. The public repository provides full source code for all of these tools, except for ATAT which one must download from its website at CalTech (due to license restrictions), though a package on the repository automates that download and compile process. A demonstration in two ternary alloy systems illustrates the capabilities of this open source stack.

10:40 AM Invited
FiPy: An Open Source Finite Volume PDE Solver Implemented in Python: *Jonathan Guyer*[1]; Daniel Wheeler[1]; James Warren[1]; [1]National Institute of Standards and Technology

FiPy <http://www.ctcms.nist.gov/fipy> is an object oriented, partial differential equation (PDE) solver, written in Python, based on a standard finite volume (FV) approach. FiPy is particularly tailored to phase transformation simulations, focusing on the phase field and level set methods. The solution of coupled sets of PDEs is ubiquitous to the numerical simulation of science problems. Numerous PDE solvers exist, using a variety of languages and numerical approaches. Many are proprietary and difficult to customize. As a result, scientists spend considerable resources repeatedly developing limited tools for specific problems. Our approach, combining the FV method and Python, provides a tool that is extensible, powerful and freely available. A significant advantage to Python is the existing suite of Open Source tools for array calculations, sparse matrices and data rendering. We will discuss our recent efforts tointegrate FiPy with one particular tool, the PyTrilinos parallel sparse solvers.

11:05 AM Invited
Implementing an Open-Source Integrated Framework for Ab Initio Thermodynamics Using Python as a Glue Language: *Raymundo Arroyave*[1]; Michael Williams[1]; [1]Texas A & M University

In this talk, I will present some recent experiences regarding the implementation of an integrated framework for ab initio calculations of thermodynamic and structural properties of crystals using Python. The open-source tools being developed are capable of seamlessly integrating a wide range of packages and programs within a single input-file based framework. Pre and post-processing of ab initio calculations using either commercial or open-source density functional theory are linked to higher level alloy thermodynamic tools, such as the ATAT Alloy Thermodynamics package, developed by Axel van de Walle to fully automate the prediction of thermodynamic and structural properties of crystals, including thermal and configurational effects. The talk will mostly consists of a brief description of the tools developed as well as their impact on the productivity of ab initio thermodynamic calculations.

11:30 AM
The 3D Materials Atlas: An Interactive Database for Materials Research: *Andrew Geltmacher*[1]; Donald Boyce[2]; Paul Dawson[2]; Matt Heying[3]; Kristina Taylor[3]; Krishna Rajan[3]; William Pearlman[4]; George Spanos[1]; [1]Naval Research Laboratory; [2]Cornell University; [3]Iowa State University; [4]Rensselaer Polytechnic Institute

The 3D Materials Atlas is an interactive, web-based repository for 3D material microstructure and property data. It has been developed as part of the ONR/DARPA "D 3-D Digital Structure" program. The goal of the atlas is to provide materials scientists the ability to store and access 3D datasets for materials research, including scientific visualization, analysis, and simulation of microstructural evolution. The atlas consists of compressed data files of experimental and computational data, a relational database, and Input/Output and plug-in interfaces used for data transfer and visualization. Examples of data currently stored in the database include 3D reconstructions of actual microstructures, statistically-based microstructural representations, material

property measurements, and computationally-derived simulation results. Novel data compression routines are used for storage and transfer of large datasets. The relational database is written using Python and PostgreSQL and allows for easy recall and search functions on any of the database fields.

11:55 AM Concluding Comments

Pb-Free Solders and Emerging Interconnect and Packaging Technologies: Electromigration, Microstructure, and Mechanical Properties

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Electronic Packaging and Interconnection Materials Committee

Program Organizers: Sung Kang, IBM Corp; Iver Anderson, Iowa State University; Srinivas Chada, Medtronic; Jenq-Gong Duh, National Tsing-Hua University; Laura Turbini, Research In Motion; Albert Wu, National Central University

Thursday AM — Room: 2020
February 19, 2009 — Location: Moscone West Convention Center

Session Chair: Nikhilesh Chawla, Arizona State University

8:30 AM

In Situ Electromigration-Induced Transient Stress in Pb-Free Sn-Cu Solder Joints Measured by Synchrotron Radiation: *Kai Chen*[1]; Nobumichi Tamura[1]; King-Ning Tu[2]; Yi-Shao Lai[3]; [1]Lawrence Berkeley National Laboratory; [2]UCLA; [3]Advanced Semiconductor Engineering

Electromigration-induced elastic hydrostatic stress in Pb-free SnCu solder joints has been studied by using in situ synchrotron X-ray white beam microdiffraction. The elastic stress within two different grains. one located at the anode end and the other at the cathode end, was analyzed based on the anisotropy of the ß-Sn crystal structure. The stress at the cathode end was almost constant except for temperature fluctuation, while the compressive stress at the anode end was build-up as a function of time in electromigration until a steady state was reached. The effective charge number of ß-Sn was estimated to be in good agreement with the calculated value. The measured compressive stress gradient is much larger than that needed in pushing Sn whisker growth.

8:45 AM

Effects of Current Stressing on Shear Properties of Sn-3.8Ag-0.7Cu Solder Joints: X. Wang[1]; Q. Zeng[1]; Q. Zhu[1]; Z. Wang[1]; *J. Shang*[2]; [1]Institute of Metal Research; [2]University of Illinois at Urbana-Champaign

Effects of electric current on the microstructure and shear properties of SnAgCu/Cu joints were investigated by lap shear of ball joints at a current density of 1.1×10^3A/cm2 and a working temperature of 83° It was found that the maximum shear load depended strongly on the current stressing time. For short durations of current stressing, only a slight decrease in the maximum shear load was observed. However, as the duration of current stressing lengthened, the maximum shear load was drastically reduced. The reductions were related to softening of the solder alloy without much loss of plasticity for the intermediate durations of current loading, and to brittle interfacial fracture at very long current loading.

9:00 AM

Direct Measure the Current Crowding Effect in Flip-Chip Solder Joints: *Shih-Wei Liang*[1]; Chih Chen[1]; K. N. Tu[2]; [1]National Chiao Tung University; [2]UCLA

As the electronic devices were concerned to have higher performance, the I/O capability should be increased. For this purpose, the numbers of solder joints need to raise and the size of solder joints need to reduced. The electromigration in the solder bumps would become an important reliability issue for this technology due to carrying high current density. The current crowding effect in flip-chip solder bumps has been reported several simulation studies. There are no experimental data to show out relation of the current crowding effect and the atom movement. In this paper, flip-chip solder bump with markers is adopted to distinguish the movement during electromigration due to current crowding effect. The marker velocity is proportional to the current density. The marker moved faster under higher current density. Also, the DZ* was obtained to be 3.34 × 10-12 cm2/s.

9:15 AM

The Effect of an Imposed Current on the Creep Rates of Sn-Ag-Cu Ball Grid Array Solder Joints: *Christopher Kinney*[1]; Tae-Kyu Lee[2]; J.W. Morris[1]; [1]University of California, Berkeley; [2]Cisco Systems

This study examines the effect of an imposed current on the steady state creep behavior of PBGA chips. These devices are subjected to loads and carry current during operational use; therefore it is important to characterize the behavior of the chip under current. The chip interconnects consist of a 4x4 grid of 610 um diameter 96.5-Sn 3.0-Ag 0.5-Cu solder balls. Different sample treatments were employed: as received, thermally aged and electromigrated. The PBGA chips were tested in creep under constant load at 20C, 75C and 100C. These conditions were repeated with the samples placed under an imposed current density to ascertain the influence of an imposed current on the creep rate. Optical and electron microscopy were used to characterize the materials before and after the tests.

9:30 AM

Electrical Conductivity Changes in Eutectic Sn-Based Solder Reaction Couples during Electromigration: Fu Guo[1]; *Jia Sun*[1]; Guangchen Xu[1]; [1]Beijing University of Technology

Electrical conductivity of electronic interconnects made with Sn-based solders undergo a significant amount of deterioration during service. With the electromigration impact, the metal atoms/ions migrated towards the direction of electron wind flow. The accumulation of atoms/ions at the anode interface could cause the hillock formation, while the depletion of atoms/ions at the cathode interface could cause the valley formation. In addition, the different a-rich and ß-rich phases in a binary eutectic system was found to separate in the bulk region of the Sn-based solders. Such mass movement will induce electrical conductivity changes at different stages of electromigration. A LabVIEW® controlled software was programmed to quantitatively measure the instantaneous electrical conductivity values after the electrical current was applied. The current study investigates the roles of different parameters, such as current density, ambient temperatures, etc., on the deterioration of electrical conductivities during the electriomigration process.

9:45 AM

Microstructure and Orientation Evolution of the Sn Phase as a Function of Position in Ball Grid Arrays in Sn-Ag-Cu Solder Joints: *Tae-Kyu Lee*[1]; Kuo-Chuan Liu[1]; Thomas Bieler[2]; [1]Cisco; [2]Michigan State University

The Thermal fatigue performance of SAC305 solder alloy joints are studied and the microstructure evolution is observed focused on Sn grain orientation during thermal cycling on thermally aged Plastic Ball Grid array (PBGA) packages. Thermally cycled PBGA packages after various pre-conditions with 196 full array solder joints are used in this study. Each selected PBGA package is polished to view the solder joints from the top by both Polarized Optical microscopy and Orientation Imaging Microscopy. The observations reveal different patterns of single and multi-grained Sn microstructure distribution as a function of position in the package depending on their pre-condition and thermal cycle history. Overall a faster degradation of thermal cycling performance is observed after aging at 100°C aging, compared to both non-aged and 150°C aged PBGAs. The difference of the distribution at different pre-conditions and evolution of the grain structures during thermal cycling are discussed.

10:00 AM

Mechanical Behavior and Corresponding Microstructural Characterization of Solder Materials: *Fang Cao*[1]; Ellen Cerreta[1]; George Gray[1]; [1]Los Alamos National Laboratory

Enhanced need for electronic devices to survive and function in extreme environments, such as conditions of stress and/or temperatures fluctuations, requires knowledge of the mechanical properties of solder materials in a wide range of temperatures and strain rates. Currently information on the dynamic response of solder alloys is limited. The focus of this study is, therefore, to investigate the mechanical behavior of three solder alloys: Sn63Pb37, Sn62Pb36Ag2, and Sn96.5Ag3Cu0.5 (wt%) at a variety of temperatures (77 ~ 298 K) and strain rates (10-3 ~ 103) by conducting quasi-static and dynamic compression tests. Microstructural characterization of these materials prior to and after testing was carried out by scanning electron microscopy (SEM) to correlate observed properties with developing microstructures. The effects of the Sn grain morphology and orientation, precipitate microstructure and corresponding substructural changes on the mechanical response of these solder alloys were studied and discussed in detail.

10:15 AM Break

10:30 AM

Effect of Microstructure Evolution on the Mechanical Properties of SAC Solder Joints: *Yan Xing*[1]; James Woods[1]; Pushkraj Tumne[1]; Michale Meilunas[2]; Peter Borgesen[2]; Eric Cotts[1]; [1]Suny-Binghamton; [2]Unovis Solutions

We examine the effect of the evolution of solder joint microstructure (Sn dendrite and precipitate size, Sn grain size and orientation) on the mechanical properties of SnAgCu solder joints. Solder joints (500 micron SAC205 balls on Cu/OSP pads) were subjected to thermal cycling or room temperature shear fatigue tests. Variations in sample lifetime with initial (as-solidified) microstructure, dwell time and evolution of microstructure were examined. Crack initiation and growth were examined as a function of dwell time, or number of shear fatigue cycles. Correlations between solder joint lifetime and microstructure were studied. We found that Sn dendrite, precipitate and grain size was all coarsened due to thermal cycling aging. The degree of recrystallization also changed as a function of dwell time. The results of both tests show that although recrystallization may help cracks propagate, cracks can form before recrystallization occurs.

10:45 AM

Effects of Microstructure on Creep of Sn-3.5Ag Solder: *Sung Bum Kim*[1]; Yu Jin[1]; [1]KAIST

Understanding the mechanism of creep deformation is an important element of estimating the solder joint life time accurately. However, in real life, creep data of Pb-free solder alloys vary widely even for a given composition. A main culprit is differences in the solder microstructure (β-Sn granular size and volume fraction, grain size, Ag_3Sn particle size and spacing), which are dependent of solidification conditions. Varying microstructures are obtained from various cooling rates from melt, steady maintaining temperatures and times during solidification process. Primary β-Sn granule is surrounded by walls of creep resistant eutectic region which is a mixture of β-Sn and precipitates of Ag_3Sn. In the present work, creep tests were conducted under uniaxial tension by using the Sn-3.5Ag alloy with varying microstructures. Based on nano-indentation measurement of β-Sn and eutectic region, a model is also presented here, which explains effects of solder microstructure.

11:00 AM

Effects of Solder Cu Concentrations on the Formation of Micro Voids: *Yi-Wun Wang*[1]; C. Robert Kao[1]; [1]National Taiwan University

In the reactions between Sn-based solders and Cu substrate, the formation of micro voids within the Cu3Sn layer had been reported by many research groups. These micro voids raise the potential of brittle interfacial fracture of the solder joints. In this study, the effect of Cu concentration in solders on the micro voids formation was studied. The solder compositions used were SnxCu (x=0~0.8 wt.%). The reflow temperature profile had a peak temperature of 235°C. The reaction times were 90 s and 30 s. The samples were then subjected to solid-state aging at 160°C for 500, 1000 or 2000 hrs. The experimental results show that the Cu concentration in solder can influence the micro voids formation. High Cu concentration in solder retards the micro voids formation.

11:15 AM

Low Stress Creep in SAC Solder: *Kathryn Baldwin*[1]; Chris Kinney[1]; Tae-kyu Lee[2]; Weidong Xie[2]; John Morris[1]; [1]University of California, Berkeley; [2]Cisco Systems

It is well known that behavior and governing equations for creep change in the low stress regime. There is also a paucity of data for Pb-free solders in the low stress creep regime. The work reported here characterizes the creep behavior for two commercially important SnAgCu solders in the low stress regime and explores the governing constitutional equations. The solder specimens were tested using constant mechanical loads under various conditions in a double-shear configuration. Both as-cast and aged specimens were tested.

11:30 AM

Effect of Strain Rate and Temperature on Tensile Properties of Sn-8.5Zn-0.5Ag-0.01Al-0.1Ga Solder: *Teng-Chun Hsuan*[1]; Kwang-Lung Lin[1]; [1]National Cheng Kung University

This study investigated the tensile properties of Sn–8.5Zn–0.5Ag–0.01Al–0.1Ga (5-e) solder alloy under various temperatures (25°C~180°C) and strain rates (8.33×10-4 s-1~3.33×10-2 s-1). The yield stress and ultimate tensile strength increase while the ductility reduces with an increase in strain rate or a lowering in temperature. Most of the fracture surfaces of 5-e alloy appear to show dimple morphology except for the case with strain rate of 3.33×10-2 s-1 at 25°C whence existing a fracture transition from ductile to brittle. During tensile test at 180°C and 8.33×10-4 s-1, the grain growth of ß-Sn caused the ductility reduction of 5-e alloy. An increase in strain rate and the lowering in temperature result in reduction in the dimension of the fracture dimple. With temperature increasing from 25 to 180°C, the strain hardening exponent (n) of 5-e solder alloy reduces gradually but the strain rate sensitivity exponent (m) increases rapidly.

11:45 AM

Re-Precipitation of Cu_6Sn_5 onto Ni Substrate during Thermal Aging of Solder Joints: *Bo-Mook Chung*[1]; Joo-Youl Huh[1]; [1]Korea University

In electronic packaging, SnAgCu (SAC) solders are commonly used to produce solder joints with Ni/Au-finished substrates. In this study, the Cu/Sn/Ni and Cu/Sn/Cu/Sn/Ni diffusion couples were employed to examine the re-precipitation of Cu_6Sn_5 particles in the bulk of a SAC solder onto the Ni substrate during solid-state aging. Pure Sn (27 μm) and Cu (0.8 μm) layers were sequentially electrodeposited on thick Ni substrates to produce the diffusion couples. The diffusion couples were aged at 200°C for different periods of time. At the early stage of aging, all the Cu layers were completely transformed into $(Cu_{1-y}Ni_y)_6Sn_5$ and a ternary $(Cu_{1-x}Ni_x)_6Sn_5$ compound layer formed at the Sn/Ni interface. The thickness and Ni content of the $(Cu_{1-y}Ni_y)_6Sn_5$ and $(Cu_{1-x}Ni_x)_6Sn_5$ layers were monitored as functions of the aging time. In this presentation, we will also discuss the formation and growth of a $(Ni,Cu)_3Sn_4$ layer at the $(Cu_{1-x}Ni_x)_6Sn_5$/Ni interface.

12:00 PM

Shear and Pull Testing of Sn3.0Ag0.5Cu Solder with Ti/Ni(V)/Cu UBM during Aging: *Kai-Jheng Wang*[1]; Jeng-Gong Duh[1]; [1]National Tsing Hua Univ

The Ti/Ni(V)/Cu under bump metallization is wildly used in the flip chip technology today. During reflow or aging, Sn atoms would diffuse to Ni(V) layer to form the Sn-rich phase, as the so-called "Sn-patch". However, the literatures about relationship between Sn-patch and mechanical property of solder joint were limited. In this study, the sputtered Ti/Ni(V)/Cu UNM was reflowed with Sn3.0Ag0.5Cu solder, and then the solder joint was aged at 125 and 200C, respectively, for 500h, 1000h, and 2000h. (Cu,Ni)6Sn5 and (Cu,Ni)3Sn formed and grew gradually at interface between solder and Ni(V) during aging at 125C. In contrast, Sn-patch replaced Ni(V) layer, and another (Ni,Cu)3Sn4 formed between (Cu,Ni)6Sn5 and Sn-patch at 200C for 1000h. After different heat treatment, the solder joints were tested by a XYZTEC bonding tester. The effects of the aging temperature and Sn-patch formation on mechanical property of the solder joint would be probed and discussed.

12:15 PM

Strain Localization in Pb-Free Solder Joints Due to Rate-Dependent Solder Behavior: *Dennis Chan*[1]; Xu Nie[1]; Ganesh Subbarayan[1]; Indranath Dutta[2]; [1]Purdue University; [2]Washington State University

Increasingly, it is necessary to understand Pb-free solder response under conditions from quasi-static office use environment to drop/shock conditions. Significant existing research is focused on SnAgCu solder behavior at low strain rates (10-6 to 10-3s-1). In a companion paper we presented data characterizing behavior at high strain rates and constitutive models valid across nine decades of strain rate. This study uses that data to numerically model strain localization in solder joints from rate-dependent loading. We demonstrate at low strain rates, plastic damage accumulation and failure is in the solder near its interface with the intermetallic compound. Consistent with experimental observations, use of rate dependent solder behavior predicts increasing load localization at the interface with increasing loading rate. We use cohesive zone fracture models embedded in finite element models to characterize rate-dependent failure at the interface. We simulate ball shear and ball pull tests to demonstrate rate-dependent behavior effects of solder.

Progress in Computational Materials Science and Engineering Education: Session II

Sponsored by: The Minerals, Metals and Materials Society, TMS: Education Committee

Program Organizers: Gregory Olson, Northwestern University; Anter El-Azab, Florida State University; Katsuyo Thornton, University of Michigan; Laura Bartolo, Kent State University

Thursday AM
February 19, 2009

Room: 3003
Location: Moscone West Convention Center

Session Chairs: Anter El-Azab, Florida State University; Katsuyo Thornton, University of Michigan

8:30 AM Invited

Molecular Simulation Modules in Undergraduate and Graduate Education: Examples from Molecular Engineering: *Aaron Keys*[1]; Christopher Iacovella[1]; Sharon Glotzer[1]; [1]University of Michigan

We discuss the use of molecular simulation modules developed using the Glotzilla simulation API in undergraduate and graduate courses teaching fundamental concepts in thermodynamics, kinetics, and molecular interactions. The API enables easy creation of MC and MD simulation modules, realtime 2-d and 3-d rendering tools, and analysis methods. The modules are coordinated with a Wiki and link to the Materials Digitial Library (MATDL) Soft Matter Wiki and digital library repository (www.matdl.org). This provides students with relevant linked material including definitions of key terms, explanations of algorithms, research examples, and links to relevant literature. As examples, we show modules on phase separation, crystallization, liquid-crystalline ordering, and polymer dynamics designed for an undergraduate course in molecular engineering at the University of Michigan. *The molecular engineering course was developed and taught by M.J. Solomon and M.A. Burns. MatDL is a collaboration between the University of Michigan and Kent State University (NSF DUE-0532831).*

8:55 AM Invited

Crystal Growth: Experimental and Mathematical/Computer Modeling Courses in Beauty, Symmetry and Complexity: *John Lowengrub*[1]; Daniel Mumm[1]; Katsuyo Thornton[2]; [1]University of California, Irvine; [2]University of Michigan

In this talk, we discuss two month-long courses on crystal growth we developed for high-school students as part of the California State Summer School for Mathematics and Science (COSMOS) at the University of California, Irvine. The first course dealt with concepts and characterization of crystal growth using physical theory and experiments. In this course, we discussed the underlying science of why crystals take their shape as well as the basics of thermodynamics, the role of atomic structure and how, together with environmental conditions, these determine the symmetry and shape of crystals. The second course focused on modeling and simulation of crystal growth at the micro and nano scales. The students applied the computer models to develop their own virtual crystals with remarkable shapes and symmetries. The students took both courses at the same time, and working in teams, produced a research project which involved both experimental and modeling components.

9:20 AM Invited

Computational Materials Science Course for Soft Matter Physicists: *Robin Selinger*[1]; [1]Kent State University

Computer simulation plays an important role in the study of soft matter, including both fundamental research and engineering applications. We describe a Computational Materials Science course at Kent State's Liquid Crystal Institute, with a focus on modeling liquid crystals and other soft materials. Topics covered include: random walks and diffusion in disordered media; Monte Carlo methods and lattice models; simulated annealing; modeling microstructure and defects in liquid crystal cells; and off-lattice molecular simulation. Models and computational algorithms are discussed in class, along with techniques for data analysis and visualization. Students then independently write their own simulation codes "from scratch" in the programming language of their choice. The final few weeks of the course are devoted to individual research projects. We present examples of lesson units with associated homework exercises, and discuss the course's long-term impact on student achievement.

9:45 AM Invited

Enhancing Materials Science and Engineering Curricula through Computation: *John Kieffer*[1]; [1]University of Michigan

Our goal is to devise a more effective instructional process by incorporating computation and cyber infrastructure (CI) throughout materials science and engineering (MSE) undergraduate curriculum. We expect students to gain a better fundamental understanding of materials science concepts and principles, and to advance their computational thinking and proficiency. To this end we are developing instructional modules that (i) visually present fundamental concepts in materials science, thereby increase student comprehension; (ii) actively engage students in computer-based experimentation; and (iii) concentrate student attention on algorithmic thinking and concepts in scientific computation. Modules are based on visualization, simulation, and numerical problem solving approaches. Currently we are establishing proof of concept in the context of the MSE Thermodynamics course by evaluating student learning before and after introducing these modules. In this presentation we demonstrate examples of such modules and report on the impact this effort has had to date.

10:10 AM Break

10:20 AM

The Role of Coaching in Facilitating Computational Materials Science Education: *Michele Manuel*[1]; McKenna Ann[2]; [1]University of Florida; [2]Northwestern University

Introduction of computational tools in the undergraduate curriculum is a daunting task. A new coaching model has been implemented in a junior-level materials science and engineering course that integrates computational tools within the framework of traditional capstone design. This model utilizes graduate students as coaches to serve as a technical resource and role model for the undergraduate design teams, producing learning experiences that are at a high technical level. Results show that successful coaching provides greater individualized attention for the undergraduate design teams and professional development opportunities for the graduate student coaches.

10:45 AM

Computational Materials Science Education as Part of a Degree Program in Computational Science: *Anter El-Azab*[1]; Sachin Shanbhag[1]; Max Gunzburger[1]; [1]Florida State University

This talk summarizes an effort to establish a Computational Materials Science (CMS) subfield in a wider-scope interdisciplinary computational science program at Florida State University, with both undergraduate and graduate components. The talk addresses the conceptual and scientific challenges that must be dealt with in order to develop and implement CMS curricula in a traditional university environment. These challenges include (i) creating the right level of synergy between CMS and other programs in engineering, chemistry, physics and computational mathematics and scientific computing, (ii) striking the right balance between various CMS program components, (iii) developing and teaching CMS curricula in way that integrates materials theory and computational techniques, and (iv) performing the task of CMS education at the undergraduate level. The relevant issues will be illustrated by three examples: advanced Monte Carlo modeling of materials, continuum models of microstructure evolution in materials, and multiscale modeling methods.

11:10 AM

Multiyear Computational Materials Design Education: *Gregory Olson*[1]; [1]Northwestern University

The Bodeen-Lindberg Materials Design Studio serves as a central teaching facility for computational MSE in the undergraduate materials curriculum at Northwestern. Software tools introduced throughout core courses are integrated in a required junior-level Materials Design course. Through an integration of education activities of the Segall Design Institute with funded design research activities of the Materials Technology Laboratory, coaching by graduate students and post-doctoral researchers facilitates cross-disciplinary concurrent computational engineering of materials and structures in engineering schoolwide "institute projects" involving multidisciplinary undergraduate teams spanning freshman to senior level. Project examples include "Civil Shield" addressing materials and structures for civilian anti-terrorism bomb mitigation, and "Smart Stent" integrating high-performance shape memory alloys in endovascular stent designs.

Computational Materials Research and Education Luncheon Roundtable: Gibbs: A Multi-Component Thermodynamics Calculation and Visualization Suite

Sponsored by: National Science Foundation
Program Organizer: Laura Bartolo, Kent State University

Thursday PM Room: 3003
February 19, 2009 Location: Moscone West Convention Center

Session Chairs: Adam Powell, Opennovation; Edwin Garcia, Purdue University; Raymundo Arroyave, Texas A & M University

12:00 PM Panel Discussion

Recycling—General Session: Session III: Aqueous Processing

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

Thursday AM Room: 2024
February 19, 2009 Location: Moscone West Convention Center

Session Chair: Jeffrey Spangenberger, Argonne National Laboratory

8:30 AM

Fundamental Aspects of Electrocoagulation: Removal of Oily Wastewaters from the Metallurgical Industry: *Mauricio Torem*[1]; Antonio Merma[1]; Rodolfo Rangel[1]; Roberto de Carvalho[1]; Lorgio Gonzales[1]; [1]Catholic University of Rio de Janeiro PUC-Rio

In this work, the electrocoagulation technique was studied in order to treat chemically stabilized concentrated oil-water emulsions. This study was mainly focused on the effects of operating parameters such as initial pH, current density, reaction time, ionic strength, electrode distance and inlet concentration on the separation of oil as measured by the chemical oxygen demand (COD) method. The synthetic emulsion was prepared from Shell - Talpa 30 oil (3g.L-1) and sodium dodecyl sulfate (1.0 g.L-1), having a Zeta potential around -70 mv at pH 8.7. The process was carried out in an electrocoagulation cell with a set of four parallel monopolar electrodes. This set consisted of two aluminum plate anodes and two 316L stainless steel plate cathodes. Kinetic curves showed that the electrocoagulation process exhibits three phases. The results showed that the period to reach the reactive phase decreased as the current density increased and the pH values decreased.

8:50 AM

Biosorption Removal of Aluminum Species from Wastewaters Streams: *Mauricio Torem*[1]; Javier Basurco[1]; [1]Catholic University of Rio de Janeiro PUC-Rio

In this work, a gram-positive bacteria was used as biosorbent to elucidate the aluminum load capacity under different conditions related to metallurgical and chemical plants. The sorption data followed the Langmuir, Freundlich, Temkin, Dubinin-Radushkevich isotherms. In order to determine the best isotherm fit, three error analysis methods were used to assess the data: correlation coefficient (R2), residual root mean square error (RMSE) and Chi-square test. The error analysis established that the Freundlich model fits better the aluminum biosorption data. The maximum sorption capacity was found to be 41.59 mg.g-1. The maximum removal of aluminum was 95% at pH around 5. Thermodynamic parameters have also been evaluated and the results show that the sorption process was spontaneous and exothermic in nature. The experimental kinetics data was evaluated considering three models (pseudo-second order, pseudo-first order and intraparticle diffusion). This study indicated that the R. opacus is an environmental friendly biosorbent.

9:10 AM

Biosorption of Cadmium from Aqueous Solutions by Waste Microzyme: *Chen Yunnen*[1]; [1]Jiangxi University of Science and Technology

The test and use of natural materials as biosorbents for the removal of heavy metals from industrial wastewater is under constant development. Consequently this work concerns the study of cadmium biosorption by means of pretreated waste microzyme. The cadmium removal study has been carried out batchwise where the influence of physico-chemical key parameters such as the pH value of solution, the temperature, the agitation speed, the contacting time, the dosage of adsorbent and initial cadmium ions concentration have been considered. The maximum percent removal was attained at the pH 7.0 after about 30 min. The adsorbent can be effectively regenerated using 0.1M HCl and reused. The experimental results provided evidence for ion exchange as the major biosorption mechanisms for binding the divalent metal ions to the waste microzyme. Waste microzyme was a potential biosorbent for the removal of Cd(II) from the effluent of electroplating industry.

9:30 AM

Effects of Organic Acids on Extraction of Cr(III) in Soils Contaminated by Chromium-Containing Slag: Youze Xu[1]; *Liyuan Chai*[1]; Zhihui Yang[1]; Shunhong Huang[1]; [1]Institute of Environmental Science and Engineering, School of Metallurgical Science and Engineering, Central South University

The effect of oxalic acid, acetic acid, citric acid and EDTA on extraction of Cr(III) in soils contaminated by chromium-containing slag were investigated using a batch of incubation experiment. The results show that the pH value decreases more obvious with the increase of the amount of organic acid. The amount of Cr(III) extracted increases with increasing the amount of organic acid. When the ratio of organic acids to total Cr(III) was 5:1, citric acid revealed the highest extraction effectiveness, followed by EDTA, oxalic acid and acetic acid, respectively. The amounts of Cr(III) extracted by citric acid, EDTA, oxalic acid and acetic acid increased by 439%, 244%, 215% and 162%.

9:50 AM

Leaching and Reduction of Cr (VI) by Indigeous Microorganism in the Contaminated Soils: Youze Xu[1]; Liyuan Chai[1]; *Zhihui Yang*[1]; Shunhong Huang[1]; Changqing Su[1]; Bing Wang[1]; [1]Central South University

The leaching and reduction of Cr(VI) in soils contaminated by chromium-containing slag were investigated with column experiments. The results showed that Cr(VI) concentration in leachate decreased from 988 mg L-1 to 407 mg L-1 after 7 days when water was used as leaching agent. However, Cr(VI) in leachate in culture medium treatment was not detected at above periods. In comparison, Cr(VI) concentration in leachate from autoclaved soil remained 398 mg L-1 at the end of experiment. The results indicated that the indigenous microorganism was capable of reducing Cr(VI). The amount of Cr(VI) reduction was 335 mg at the whole experiment period and the reduction rate was 67.09 mg d-1. Carbon supply showed minor effect on Cr(VI) reduction. However the reduction capability of Cr(VI) could be improved by combination of the carbon and the nitrogen. The optimal quantity was 5 g L-1 of yeast extract and 4 g L-1 of glucose.

10:10 AM

Effects of the Mixed Surfactants on Detoxification of Chromium-Containing Slag by Achromobacter sp. CH-1: Lijuan Chen[1]; *Liyuan Chai*[1]; Yan Huang[1]; Yude Shu[1]; [1]School of Metallurgical Science and Engineering, Central South University

During the detoxification of chromium-containing slag by Achromobacter sp. CH-1, anionic surfactant Sodium Dodecyl Sulphate(SDS) and its mixed systems with different Tween surfactants(Tween 20, Tween 60 and Tween 80) were used to promote the interaction between the bacteria and the chromium-containing slag and the rate of acid-soluble Cr(VI) leached from the slag. The effects were evaluated by the surface tension, the pH of the leaching solution and the leaching rate of total Cr(VI) from the slag. The results showed that the surfactants systems improved Cr(VI) leaching and its detoxification of chromium-containing slag. The mixed surfactants of SDS combined with Tween surfactant revealed better effectiveness of detoxification than SDS only. When the mass ratio of SDS to Tween 80 was 1:1, the rate of Cr(VI) leached from the slag increased by 12%.

10:25 AM Break

10:40 AM

Adsorption of Copper from Aqueous Solution by Chemically Modified Orange Peel: Sha Liang[1]; Ningchuan Feng[1]; Qinghua Tian[1]; *Xueyi Guo*[1]; [1]School of Metallurgy Science and Technology

In this study, adsorption of copper by chemically modified orange peel was investigated. A conspicuous change occurs in the surface morphology of the biomass due to modification, which is depicted by SEM images. Equilibrium isotherms and kinetics were obtained, and the effects of various factors, including solution pH, contact time, initial metal ions concentration and temperature, were studied by batch experiments. Equilibrium was better described by Langermuir isotherms rather than Freudlich isotherms, and maximum adsorption capacity was 70.67mg•g-1. With increase of temperature, adsorption efficiency decreased. The biosobent was suitable for repeated use for more than five cycles.

10:55 AM

Adsorption of Copper Ions in Aqueous Solution by a Submersed Aquatic Macrophyte Potamogeton Pectinatus L: Licheng Zhou[1]; *Liyuan Chai*[1]; [1]Central South University

The use of aquatic plants for the removal of heavy metals from wastewater has gained high interest. In this study, batch experiments were conducted to evaluate the adsorption of copper ions in aqueous solution by P. pectinatus L. under various conditions of contact time, initial pH of the solution, metal concentration and adsorbent dosage. The results showed that the maximum adsorption amount of copper ions by P. pectinatus L. was 22.60 mg g-1 when the initial copper ions concentration was 98.41mg L-1 at pH 4.5. The Langmuir and Freundlich models were used to describe the adsorption equilibrium of copper ions on P. pectinatus L. and the adsorption followed the Langmuir isotherm. The adsorption kinetic was well-fitted with pseudo-second-order sorption equations.

11:10 AM

Novel Technology for Treatment of Acidic Wastewater Containing Mercury in Zinc Smelter by Biologics: Qingwei Wang[1]; *Liyuan Chai*[1]; Yunyan Wang[1]; Qingzhu Li[1]; Yude Shu[1]; [1]School of Metallurgy Science and Engineering, Central South University

This study focused on acidic wastewater from producing sulfuric acid system in zinc smelter containing mercury 21.48mg/L,zinc 55.85mg/L, lead 38.50mg/L, copper 1.68mg/L, cadimun 10.25mg/L, As 29.86mg/L treated by biologics. The factors of pH value, the ratio of biologics to mercury, complexing time, hydrolytic time and temperature was studied in this paper. Experimental results indicated that at pH value 10, quantity of biologics to mercury ratio was 16, complexing time 30min, hydrolyzation time 20min, temperature at 40°, concentration of mercury in treated water was removed to 22.15µg/L. At same time heavy metals such as Zn, Pb, Cu, Cd, As was removed by biologics, the remained concentration in treated water was Zn 0.53mg/L, Pb 0.12mg/L, Cu 0.01mg/L, Cd low to 0.01mg/L and As 0.023mg/L. According to EDAX analysis, mercury content in complexing sediment reached 28.49% easily to recycle as raw material and low concentration of heavy metals in hydrolytic sediment easily to dispose and treat.

11:25 AM

Removal of Hg(II) from Aqueous Solutions Using Spent Grain: *Liyuan Chai*[1]; Qingzhu Li[1]; [1]Central South University

In this study, spent grain was used as an adsorbent for the removal of Hg(II) from aqueous solutions, the process parameters such as contact time, solution pH, adsorbent dose, and initial Hg(II) concentration were studied in batch experiments. The initial adsorption process was fast, 91.08% of adsorption occurred within 5 min and equilibrium was reached at around 30min. Adsorption process was found to follow pseudo-second-order kinetics. The equilibrium data were better fitted to Langmiur isotherm than Freundlich isotherm with the maximum adsorption capacity 41.36 mg/g. The structure and component of spent grain before and after adsorption of Hg(II) were investigated using scanning electron microscope(SEM) and energy dispersive X-ray analysis(EDAX), these analysis also confirmed the adsorption of Hg(II) onto spent grain. The results indicated that spent grain had potential as a new inexpensive adsorbent for Hg(II) removal from aqueous solutions.

11:40 AM

Adsorption and Recovery of Ag(I) from Aqueous Solutions Using Spent Grain: Qingzhu Li[1]; *Liyuan Chai*[1]; [1]Central South University

The brewing industry byproduct, spent grain(SG), was evaluated for its ability to adsorb Ag(I) from aqueous solutions. Ag(I) adsorption was dependent on solution pH, contact time, adsorbent dose, initial Ag(I) concentration and temperature. The kinetic data was well described by pseudo-second-order kinetic model, indicating that chemical adsorption was the rate-controlling step. The equilibrium data followed Freundlich isotherm rather than Langmuir isotherm, suggesting heterogenity of the adsorption sites on spent grain. Ag(I) desorbed from Ag(I)-loaded spent grain was also evaluated in this study. HCl, NaOH, Na2S2O3 and ultrapure water were chosen as eluants and desorbed Ag(I)-loaded spent grain for 30min, Ag(I)-loaded spent grain desorbed in 0.1M Na2S2O3 exhibited higher elution efficiency as compared with other eluants. The results indicated that application of spent grain for adsorption and recovery of silver from aqueous solutions was feasible.

11:55 AM

Treatment of Wastewater Containing Benzene by Technology Combined Blow-off with Fenton Reagent Oxidation: *He Dewen*[1]; Qin Yan[1]; Liang Ding-ming[1]; Wang Wei-liang[1]; Du Lu[1]; [1]Central South University

The influence of wastewater containing benzene from chemical industry by technology combined blow-off with Fenton reagent oxidation was experimentally studied. The present results suggest that the technology combined blow¬-off with Fenton reagent oxidation can effectively remove benzene pollutant in wastewater. The main factors that influence the removal benzene such as temperature and blowing time and volume, pH and reagent dosage of H2O2 and Fe2+ are studied and the optimal experimental conditions are as follows: time 20min, temperature 40°, air-blowing volume 0.4L/min, pH value 5, and H2O2 and Fe2+ dosage 2mL/L and 200mg/L respectively. Under the above conditions, benzene pollutant can be removed up to 97%. Compared to other removal ways of wastewater containing benzene, the technology combined blow-off with Fenton reagent oxidation is more effective and has the advantage of high speed.

12:10 PM

Removal of Zinc and COD from Electroplating Effluent Using Sawdust: *Chen Yunnen*[1]; [1]Jiangxi University of Science and Technology

This work concerns the removal of zinc(II) and COD by means of sawdust obtained as a by-product from locally used wood. The zinc(II) and COD removal study has been carried out batchwise where the influence of physico-chemical key parameters such as tree species, the pH value of solution, the temperature and the contacting time and dosage of adsorbent have been considered. The maximum percent removal was attained at pH 9.0 all for Zn(II) and COD after about 30 min. The adsorbent can be effectively regenerated using 0.1M HCl. The experimental results provided evidence for ion exchange as the major adsorption mechanisms for binding the divalent metal ions to the sawdust. Pine sawdust was a potential adsorbent for the removal of Zn(II) from the effluent of electroplating industry.

RPV Embrittlement and Fusion Materials: Measuring, Modeling and Managing Irradiation Effects: Fusion Reactor Materials: Technical Contributions of Professor G. Robert Odette

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS/ASM: Nuclear Materials Committee

Program Organizers: Matthew Alinger, GE Global Research; Kurt Edsinger, Electric Power Research Institute; Roger Stoller, Oak Ridge National Laboratory; Brian Wirth, University of California, Berkeley

Thursday AM — Room: 2008
February 19, 2009 — Location: Moscone West Convention Center

Session Chairs: Matthew Alinger, GE Global Research; Kurt Edsinger, Electric Power Research Institute

8:30 AM Invited

Great Footprints toward Viable Fusion Materials: The Roadmap of Professor Bob Odette: *Hideki Matsui*[1]; [1]IAE Kyoto University

UCSB is recognized worldwide for materials science excellence, and Professor Bob Odette is the main engine in nuclear materials. My interactions and collaborations with Prof. Odette have focused on the development of vanadium-based alloys for fusion reactor materials, the development of small specimen test technology to minimize the volume of materials to be irradiated

in the International Fusion Materials Irradiation Facility, and the evaluation of the Master Curve Shifts Method for predicting shift of the Ductile to Brittle Transition Temperature. These are just a small fraction of his accomplishments. More recently, he developed the "Injector Foil" experiment for helium effects in ferritic steels. His success is not only in the technical but also in education, including mentoring a number of brilliant young Japanese and European Scientists. It is difficult to cover all aspects of his influence but I will highlight some of his important accomplishments related to fusion materials.

8:50 AM Invited
Integration of Modeling and Experimental Validation in Fusion Materials Research: *Steven Zinkle*[1]; [1]Oak Ridge National Laboratory

Throughout his distinguished research career, Bob Odette has been a champion for utilization of tightly integrated physics-based models and experimental tests of model alloy systems. This efficient scientific methodology has proved particularly useful for investigating fundamental radiation effects mechanisms for materials exposed to the intense high-energy neutron irradiation environment of proposed future fusion energy systems. In this talk, a brief overview will be given to summarize current understanding of physical mechanisms responsible for void swelling and fracture toughness embrittlement of potential structural materials systems for fusion energy. The key role of the high transmutant helium generation levels in the deuterium-tritium fusion reaction environment will be discussed. Due to limited volumes of material or irradiation space, it is often essential to utilize innovative miniaturized specimen test techniques to extract the maximum useful information from nonstandard specimen geometries.

9:10 AM Invited
Understanding and Managing the Effects of Helium on Fusion Structural Material Properties: *Richard Kurtz*[1]; [1]Pacific Northwest National Laboratory

A unique aspect of the fusion neutron environment is substantial production of gaseous transmutation products such as helium and hydrogen. Helium is particularly detrimental to mechanical performance because it is insoluble in materials and can agglomerate at grain boundaries. Professor G. Robert Odette has made substantial contributions for almost 40 years to the understanding of how helium interacts with microstructural features and to the creation of more helium tolerant materials. This paper highlights his many technical contributions to understanding and managing helium effects, among which are models of the transport and fate of helium and prediction of the critical bubble size for break-away void swelling, design and implementation of novel irradiation effects experiments, including a 'helium-implanter layer' technique that enables exploration of microstructural evolution at fusion relevant He/dpa ratios, and development of advanced nanostructured ferritic alloys that offer the potential for improved radiation resistance and tolerance for high helium concentrations.

9:30 AM Invited
In Situ He Implanter Studies of the Transport and Fate of Helium at Fusion Relevant Helium to Displacement Per Atom Ratios: *Takuya Yamamoto*[1]; G. Robert Odette[1]; Danny Edwards[2]; Pifeng Miao[1]; Richard Kurtz[2]; Peter Hosemann[3]; Stuart Maloy[3]; [1]University of California, Santa Barbara; [2]Pacific Northwest National Laboratory; [3]Los Alamos National Laboratory

Thermal neutron 58-Ni reactions in NiAl layers irradiated in the JP26 and 27 HFIR experiments were used to implant alpha particles into a large matrix of iron based alloys to a depth of 6 to 8 μm. Fast neutrons generated displaced atoms at a He/dpa ratio that was controlled by the thickness of the NiAl layer for irradiations from 300 to 500°C up to over 20 dpa and 1000 appm He. We summarize some initial TEM results from these experiments, with particular emphasis on comparisons of 9 Cr tempered martensitic steels (TMS) and nanostructured ferritic alloys (NFA). A bimodal distribution of bubbles and voids is observed in the TMS. The bubbles primarily nucleate on dislocations, interfaces and grain boundaries; the bubble concentration increases at higher dislocation densities. In contrast the bubbles are much smaller in NFA and primarily form on Y-Ti-O enriched nanofeatures, rather than dislocations or interfaces.

9:50 AM Invited
Experiments and Modeling of Thermal Desorption of Helium-Implanted Iron in a Broad Temperature Regime: *Donghua Xu*[1]; Brian Wirth[1]; [1]University of California, Berkeley

Helium effects on the microstructural evolution and mechanical properties of structural materials are among the most challenging issues facing fusion materials research. Thermal helium desorption spectroscopy, through measuring He surface outflux as a function of temperature (or time), provides indirect information about the kinetics and energetics of helium transport and trapping which is important for developing a predictive model for the life performance of fusion reactors. Nevertheless, the experiments and the data interpretation are not straightforward, particularly when a wide temperature range is concerned. In this work, we present desorption data for single and polycrystalline iron implanted with 4He under varying conditions. We also present a temporally and spatially dependent rate theory model, which incorporates diffusion, trapping, detrapping, and cluster coalescence kinetics during both implantation and post-implantation thermal annealing. Both the experiments and simulations are performed over a broad temperature regime from room temperature up to BCC-FCC transformation.

10:10 AM Invited
Atomistic Modeling of Helium Interactions with Dislocations, Grain Boundaries and Coherent/Semi-Coherent Interfaces in Alpha-Iron: *Howard Heinisch*[1]; Richard Kurtz[1]; Fei Gao[1]; [1]Pacific Northwest National Laboratory

Neutron capture reactions in fusion reactor structural materials will produce high concentrations of helium that may severely degrade their creep-rupture and fracture properties if it aggregates at grain boundaries to a sufficiently high level. Mitigation of deleterious helium effects by alloy design requires detailed knowledge of the transport and fate of helium to sinks. To address these issues atomic-scale modeling methods are being used to study the fate of helium in the neighborhood of dislocations, grain boundaries and coherent/semi-coherent interfaces in alpha-iron. Results of molecular statics models show that the binding energies of helium to these defects are strongly correlated with excess atomic volume. Long-time molecular dynamics and the dimer saddle point search method indicate that interstitial helium atoms and helium-vacancy complexes are attracted to and easily migrate within dislocations and grain boundaries. The effects on the results of using different interatomic potentials will also be discussed.

10:30 AM Break

10:50 AM Invited
Nanostructured Ferritic Alloys: The Technical Contributions of Professor G.R. Odette: *Matthew Alinger*[1]; [1]GE Global Research

Oxide dispersion strengthened (ODS) ferritic/martensitic steels, have long been considered candidates for advanced fusion and fission reactor structural materials. Extensive studies in the US breeder reactor program showed that ODS alloy MA957 has high tensile and creep strengths and unusual resistance to radiation damage. Further investigation revealed that MA957 contains ultrahigh densities of stable, nm-scale features (NFs). Building on a career dedicated to understanding the causes and consequences of irradiation damage, Odette was responsible for realizing the unique opportunity to design a microstructure with the 'key ingredients' for irradiation-resistance: a) high, stable dislocation sink strengths and large numbers of stable, nm-scale features trapping He in fine-scale bubbles, b) high creep strength. Thus, research focused on understanding alloy and processing variables to optimize NF formation, mechanical properties and, thermal and irradiation stability NFs. This international effort has led to the emergence of a new class of materials, Nanostructured Ferritic Alloys (NFAs).

11:10 AM Invited
Analysis of Hardening Limits in Oxide Dispersion Strengthened Steel: *Amuthan Ramar*[1]; Robin Schaeublin[1]; [1]CRPP - EPFL

Oxide dispersion strengthened (ODS) ferritic / martensitic (F/M) steels are considered as promising materials for high temperature applications in the future fusion reactor. Oxide dispersion in steel increases the strength of the matrix at the expense of its ductility. In this paper, the hardening due to the dispersed oxide particles as a function of particle size and spatial distribution in EUROFER97 matrix were investigated. Also the impact of the alloy production steps such as ball milling and HIPping over the alloy hardening were investigated in detail. Ti addition helps in refining the size of the dispersed yttria particle by the formation of Y-Ti oxide partilces. During TEM in-situ heating up to 1000°C yttria dispersion remains unaltered, whereas dissolution is observed in the case Ti is added. Analysis of hardening using the dispersion barrier-strengthening model shows that hardening due to dislocations overcomes the one of oxides, depending on the heat treatment.

11:30 AM Invited
Constitutive Behavior Modeling of bcc Metals and Alloys before and after Neutron Irradiation: *Philippe Spatig*[1]; [1]CRPP-EPFL

In this paper we will review the development and current state of the physically-based models of plastic deformation of bcc metals and structural

alloys for nuclear applications, including the low-alloyed reactor pressure vessel steels, the high-chromium tempered martensitic steels and vanadium alloys. We will focus on the evolution of the plastic flow properties associated with the neutron irradiation temperature regime leading to hardening. The models developed to rationalize the synergistic effects of the irradiation parameters (temperature, flux, fluence) and of the metallurgical variables (chemical composition, thermo-mechanical processing) will be presented. The multi-scale nature and complexity of the processes controlling the plastic flow in technical alloys will be highlighted starting from the production and accumulation of irradiation-induced defect clusters in the matrix, followed by the interaction of the moving dislocations with those defects, leading ultimately to changes in the macroscopic plastic flow curves and subsequent degradation of the associated fracture properties.

11:50 AM Invited

Micromechanical Testing of Self-Ion Irradiation Effects in Fe-Cr Alloys: Fiona Halliday[1]; Laurence Whyatt[1]; David Armstrong[1]; *Steve Roberts*[1]; [1]University of Oxford

Fe-Cr alloys up to 12% Cr were irradiated using Fe ions to damage levels up to 5.5dpa. The effects of irradiation on mechanical properties were studied by nanoindentation and by a micro-mechanical test technique. Micron-scale cantilever test specimens were cut from the radiation-damaged surface layers, and tested in bending using an AFM/nanoindenter as an imaging/loading device. Nanoindentation tests found increases in near-surface hardness due to irradiation. The micromechanical tests found significant changes in elastic modulus, yield stress and work-hardening behaviour, varying strongly with irradiation dose and chromium content. Results will be reported, and the applicability and interpretation of these test methods discussed.

12:10 PM Invited

The Dose Dependence of Fracture Toughness of F82H Steel: *Mikhail Sokolov*[1]; Hiroyasu Tanigawa[2]; G. Robert Odette[3]; Takuya Yamamoto[3]; Takanori Hirose[2]; Nariaki Okubo[2]; [1]Oak Ridge National Laboratory; [2]Japan Atomic Energy Agency; [3]University of California, Santa Barbara

The advanced ferritic-martensitic steel F82H is a primary candidate low-activation material for fusion applications. Fracture toughness specimens of this steel were irradiated in High-Flux Isotope Reactor to a wide range of doses from 3.5 to 25 dpa. The range of irradiation temperature was from 250C to 500C. This paper summarizes the changes in fracture toughness transition temperature and decrease in the ductile fracture toughness as result of various irradiation conditions. It is shown that in the 3.5 to 25 dpa dose range, irradiation temperature plays the key role in determination of the shift of the transition temperature. At a given irradiation temperature, shift of the fracture toughness transition temperature increases slightly with dose within the studied dose range. It appears that main gain in transition temperature shift occurred during initial ~5 dpa of irradiation. The present data are compared to the available published trends.

Surface Structures at Multiple Length Scales: Surface Deposition and Properties

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS: Surface Engineering Committee
Program Organizers: Arvind Agarwal, Florida International University; Sudipta Seal, University of Central Florida; Yang-Tse Cheng, University of Kentucky; Narendra Dahotre, University of Tennessee; Graham McCartney, University of Nottingham

Thursday AM Room: 3011
February 19, 2009 Location: Moscone West Convention Center

Session Chair: To Be Announced

8:30 AM

Modulated Epitaxial Growth of Fe/Cu Nanometer-Scale Multilayers on Si Substrates Deposited by Magnetron Sputtering: J. Gao[1]; Z.P. Zhang[1]; Z.L. Wu[1]; *M.K. Lei*[1]; [1]Surface Engineering Laboratory, School of Materials Science and Engineering, Dalian University of Technology

Fe/Cu nanometer-scale multilayers of nominal modulation wavelength of 5 nm were deposited by magnetron sputtering on Si(100) substrates. Microstructure and morphology of the multilayers were examined by small/wide angle x-ray diffraction (SA/WAXRD) and cross-sectional transmission electron microscopy (XTEM), respectively. The Fe(110) and Cu(111) textures formed in the multilayers with the modulation wavelength of about 5 nm. The sharp interfaces in the epitaxial multilayers were obtained with no interfacial phase. The metastable f.c.c.-Fe and b.c.c.-Cu under the duplex modulation in composition and structure coexisted in the multilayers due to an alternatively growth by order of b.c.c.-Fe/b.c.c.-Cu/f.c.c.-Cu/f.c.c.-Fe. A critical point in the phase stability diagram as a function of modulation wavelength and atomic volume fraction was found to predict the phase states of Fe/Cu multilayers. The interface roughness and the constraint of underlayer atoms led to the phase transformation of Fe and Cu from bulk stable to metastable in Fe/Cu multilayers.

8:50 AM

Preparation of Carbon Foam Electrodeposited with Lead for the Application on Positive Current Collector for Lead Acid Batteries: *Li-Wen Ma*[1]; Bai-Zhen Chen[1]; Ya Chen[1]; Yong Pan[1]; [1]Central South University

Carbon foam may be used as current collector for lead acid batteries and reduce the weight of them. Because of the premature oxygen evolution on it, carbon foam is unable to serve as positive current collector. To use this novel carbon foam as positive current collector for lead acid batteries, the modification of lead electrodeposition is necessary. A complex system and a fluoborate system are suggested, respectively, to acquire a dense and uniform lead coating which can restrain the oxygen evolution. The morphology of lead deposit show that adopting a fluoborate system, the qualified lead deposit can be obtained. The experimental parameters like lead concentration, temperature and current density in the preparation of lead electrodeposited carbon foam from fluoborate system, have been investigated. A lead acid battery with the lead electrodeposited carbon foam as positive current collector can exhibit favorable performance.

9:10 AM

Study of Nano-TiN Composite Coating on Aluminum Alloys Strengthened by Plasma Arc: *Shiqiang Qian*[1]; [1]Shanghai University of Engineering Science

Using a combination of high speed jet electrodeposition and plasma arc quenching, a nano-TiN composite coating can be produced. The coating possess high hardness, distinctive corrosion-resistance, high bond strength and well oxidization-resistance at high temperature. Nano-TiN composite coating with fine and uniform microstructure could be prepared by the optimal process. The hardness of the nano-TiN composite coating after scanned by plasma arc was increased. The influences of TiN content on the bone strength of nano-TiN composite coating also increased because of plasma arc scanning. After scanned by plasma arc the coating's bone strength was enlarge as nano-TiN content heighten in composite coating. The plasma arc scanning also change the influences of TiN content on the corrosion resistance of nano-TiN composite coating. The corrosion resistance of coating is enhanced after scanned by plasma arc but it was on the contrary before scanned.

9:30 AM

Electroless Nickel Plating on Mg-Li Alloy by Two-Step Process: *Binna Song*[1]; Guangchun Yao[1]; Hongjie Luo[1]; Yihan Liu[1]; Zhongsheng Hua[1]; [1]Northeastern University

This paper introduces two-step process for electroless plating technology of Mg-Li alloy by nickel which purpose is to avoid the corrosion of SO42- to Mg-Li alloy and reduce the cost. Firstly, the samples pre-treated were pre-plated in NiCO3•2Ni(OH)2•4H2O solution, and then plated in the solution with NiSO4•6H2O as the main salt to form a thin film of Ni-P alloy plate. The surface morphology, structure and corrosion resistance of the coatings were studied. Results showed that a flat, bright and compact plating layer well-combinded with the base metal was obtained. The P content reached 13.56wt.%. The hardness value of the Ni-P coatings was about 549HV. Polarization curve showed that the open-circuit potential for the Ni-P film had reached -0.249V(SCE). Long passivation region was found on the polarization curve, which showed excellent anti-corrosion property of the film.

9:50 AM

Surface Morphology of Precious-Metal Free Copper Electroless Plating Process Carbon Fiber: *Dehui Che*[1]; Wei Kang[1]; Guangchun Yao[1]; Zhuokun Cao[1]; Hua Zhang[1]; [1]Northeastern University

This paper studied different Surface morphology of carbon fiber in the process on the nickel salt activated carbon fiber electroless copper plating. Before electroless plating, the pretreatment of carbon fiber is a very important

aspect. The pretreatment processing of carbon fiber including to degumming, to coarsening, to activation, to reducing four steps. In the first stage unglued studied on the tensile-strength of carbon fiber changes, with different temperature and different heating time. The Surface morphology of carbon fiber was characterized by scanning electron microscope (SEM). The results showed that carbon fiber in more than 400°C heat, Surface morphology seriously damaged. And the tensile strength decreased significantly. In the activation process, studied the formation mechanism of nickel particles on the carbon fiber. The Surface morphology of copper coating was characterized by scanning electron microscope (SEM) and Infrared Spectrometer. Further identify the nickel seeds are catalyzer for electroless plating process.

10:10 AM Break

10:20 AM

Synthesis and Electrochemical Characteristics of SnO_2-Coated $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ Cathode Materials for Lithium Ion Batteries: *Ping Yang*[1]; Chuang-fu Zhang[1]; Jing Zhan[1]; You-qi Fan[1]; Jian-hui Wu[1]; [1]Central South University

$LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ cathode materials have been coated with SnO_2 (3% wt) by heterogeneous nucleation process to improve its electrochemical performances and the physical and electrochemical properties were studied. The scanning electron microscope (SEM) images show that there is a uniform coating on the modified materials and the X-ray diffraction (XRD) patterns show that the structure of $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$is not affected by the SnO_2 coating. The electrochemical tests indicate that the SnO_2-coated $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$improves the cyclic performance and rate capability comparing the bare $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$. The electrochemical impedance spectroscopy (EIS) studies suggest that the presence of a thin SnO_2 layer could suppress the reaction between the cathode and electrolyte, and remarkably decreases the charge transfer resistance, which is attributed to the improvement in electrochemical performances.

10:40 AM

The Effect of Pre-Phosphating of Stainless Steel 316L on Adhesion of Alumina Coating: *Ali Akbar Oskuie*[1]; Abdollah Afshar[1]; [1]Sharif University of Technology

In this study stainless steel 316L has been pre-phosphated by electrochemical method and then a multi-layer coating of alumina has applied on them from a sol prepared by Yoldas process. It was believed that pre-phosphating would give a rougher surface and so a stronger physical bond between the subsequent ceramic layers would be formed. Our research reveals that although pre-phosphating produces a more cracked surface compared to the untreated steel, it improves the adhesion of the ceramic layer to the substrate. SEM, EDS, nano scratch test, and potentiodynamic corrosion tests were used to assess the effects of the prephosphating on alumina coating applied on stainless steel substrate.

11:00 AM

Three Cation Phosphating of Mild Steel: *Mohammad Zareii*[1]; Abdollah Afshar[1]; [1]Sharif University of Technology

In this study the effects of addition of calcium and nickel ions have been studied on low zinc phosphating process of St14 steel. Firstly the composition of the bath was optimized along with the temperature and pH of the bath. Then nickel nitrite has been introduced to produce the three cation phosphated layer. In this research weight of the phosphate layer and its thickness was measured in different bath compositions. For chemical and structural analysis SEM, EDX, XRD and atomic absorption was used. To prove the beneficial effects of the three cation coating compared to two cation and single cation phosphates corrosion tests has performed on the samples. Nickel and calcium ions on one hand increase the corrosion resistance of the steel and on the other hand give out a smoother phosphated layer which is a better substrate for electrophoretic painting.

11:20 AM

Evolution of Zinc-Nickel Alloy Electrodeposited Coatings with DC and Pulse Currents: *Masoud Toghraie*[1]; Mohammad Mosavie Khoei[1]; Gholamreza Heidari[1]; [1]Amirkabir University of Technology

New electrodeposition processes of zinc-nickel alloys such as pulsed electrodeposition have been producing deposits with better physical and anti-corrosion characteristic.In this research chloride bath was used and Zn-Ni alloy deposits were obtained using direct and pulse currents. The taguchi statistical method was used for experiment planning and optimization. Pulse current seems to increase brightness and percentage of nickel in the deposits. In addition, the polarization curve of zinc-nickel deposits with pulse current is shifted to positive potentials in comparison with direct current curves. The morphology of surface coatings was examined by means of metallography observations and scanning electron microscopy methods. The temperature of plating bath had a very strong effect on the composition and microhardness of coating. Frequency had a little effect on chemical composition but considerable effect on CCE.

Transformations under Extreme Conditions: A New Frontier in Materials: Driven Reactions

Sponsored by: The Minerals, Metals and Materials Society, ASM International, ASM Materials Science Critical Technology Sector, TMS Materials Processing and Manufacturing Division, TMS/ASM: Phase Transformations Committee
Program Organizers: Vijay Vasudevan, University of Cincinnati; Mukul Kumar, Lawrence Livermore National Laboratory; Marc Meyers, University of California-San Diego; George "Rusty" Gray, Los Alamos National Laboratory; Dan Thoma, Los Alamos National Laboratory

Thursday AM — Room: 3001
February 19, 2009 — Location: Moscone West Convention Center

Session Chairs: Vijay Vasudevan, University of Cincinnati; Mukul Kumar, Lawrence Livermore National Laboratory

8:30 AM Invited

In Situ XRD Studies of Self-Propagating Formation Reactions in Steep Thermal and Chemical Gradients: *Timothy Weihs*[1]; [1]Johns Hopkins University

Exothermic formation reactions are known to self-propagate in multilayer foils with nanoscale layers. These foils typically contain hundreds or thousands of nanoscale layers, and the layers alternate between materials with large, negative heats of mixing. Ni/Al, Ti/B, Nb/Si and Ti/C are some simple examples. The exothermic reactions can travel at velocities greater than 30 m/s and they can reach temperatures as high as 3300 K. The combination of rapid propagation and high temperatures produces extremely fast heating rates (~10^7 K/s) within the reaction front, while the nanoscale layers provide very steep chemical gradients. Here we investigate the impact of both extremes (heating rate and chemical gradient) using ex situ and in situ X-ray diffraction experiments on Ni/Al and Ni/Zr multilayer foils. The sequences of phase transformations that appear under fast and slow (~1 K/s) heat rates are shown to be different and the impact of steep chemical gradients is assessed.

9:05 AM Invited

Intermetallic Reactions under Extreme Strain Rate Conditions: Instrumented Experiments and Meso-Scale Simulations: *Naresh Thadhani*[1]; [1]Georgia Institute of Technology

The occurrence of intermetallic reactions in powder mixture compacts and laminates of foils, under extreme strain-rate conditions generated with uniaxial strain and uniaxial stress gas gun experiments will be described. The discussion will be based on in-situ time-resolved measurements employing stress gauges, velocity interferometry, and high-speed digital imaging to measure the stress profiles, shock velocity, and transient deformation states. Meso-scale simulations of shock-wave propagation through discretely represented constituents (with imported microstructures) performed using CTH code to investigate the effects of reactant morphology on deformation and mixing of reactants in dense powder compacts and foils, will also be described. The results reveal the heterogeneous nature of shock waves propagating through the reactants of dissimilar physical and mechanical properties, and resulting in localized flow, jetting, and vortex formation, prior to reaction initiation. The information generated is useful for understanding the reaction mechanisms and controlling their initiation and resulting energy release.

9:40 AM

Reaction of Ni-Al Laminate Composites by Laser Shock Compression and Spalling: *Chung-Ting Wei*[1]; Marc Meyers[1]; Vitali Nesterenko[1]; Brian Maddox[2]; Timothy Weihs[3]; [1]University of California, San Diego; [2]Lawrence Livermore National Laboratory; [3]Johns Hopkins University

A new reactive laminate material was developed, which consists of alternate layers of Ni and Al with bi-layer thickness of of 8.3 and 48 μm. Their potential in tailoring the energy release upon impact was investigated by extreme laser loading. The laser energy was varied between 100J (initial estimated pressure

P~140 GPa) and 400 J (P~350 GPa) with an initial duration of 3 ns. SEM, EDX and optical microscopy were carried out on the samples to study the damage induced, failure modes, and spall due to the laser interaction. It was found that the 8.3 μm laminate exhibited localized interfacial reaction at both laser energies. Potential reaction products of Ni and Al are Ni3Al, NiAl3, Ni2Al3, and amorphous Ni-Al structure, analyzed by X-Ray diffraction pattern. The cooling rate is 5.7×105 K/s and cooling time is 2.1ms approximately, by calculating from the secondary dendrite arm spacing of the reaction products.

10:00 AM

Explosive Consolidation of Ti-6Al-4V Powder: A Structure-Property Reference for Rapid-Layer Manufacturing Using Ti-6Al-4V Powder: *Noe Alba-Baena*[1]; Lawrence Murr[2]; Carlos Ramirez[3]; José Olivas Pro[1]; [1]Universidad Autonoma de Ciudad Juarez; [2]University of Texas; [3]Delphi

Rapid-layer manufacturing or rapid prototyping (RP) based upon liquid-phase sintering or melting of metal or alloy powders by electron or laser beams features the prospect for performance optimization through process-determined structure-property optimization. In contrast to wrought or cast Ti-6Al-4V where yield strengths average ~1 GPa with elongations ranging from 4-14%, RP technologies produce products with yields strengths above 1.2 GPa and elongations as high as 25%. Hardnesses have been observed to vary from HRC 36 to 50 in contrast to wrought hardnesses of HRC 37. But shock loaded, bulk Ti-6Al-4V has demonstrated hardnesses in excess of HRC 50. In this research RP Ti-6Al-4V powder ~30 μm) was explosively consolidated into a monolithic rod from which tensile specimens and hardness coupons were extracted along with sections utilized for optical and electron microscopy. The microstructures and mechanical properties were compared with those for electron beam RP for the same Ti-6Al-4V powder.

10:20 AM

High-Energy-Density Structural Energetic Materials Using Linear Cellular Alloy Exoskeletons: Naresh Thadhani[1]; *Joe Cochran*[1]; Tammy McCoy[1]; Anthony Fredenburg[1]; [1]Georgia Institute of Technology

We are investigating the design, fabrication, and evaluation of high-We are investigating the design, fabrication, and evaluation of high-energy-density structural energetic materials, based on coupling of intermetallic- and thermite-forming reactive powder mixtures with Linear Cellular Alloys (LCAs). The LCAs, made as honeycomb structures from powder extrusion and reactive sintering, are used as aerodynamic casings (exoskeletons) for ballistic delivery of energetic materials. LCA casings are being made from high-strength steels, high-density Ta and Ta matrix composites. The honeycomb casings are to be filled with highly-exothermic intermetallic (ie Ti, Si) and thermitic (e.g., Ta+Fe2O3) micro- and nano-scale powder mixtures. The focus is on manipulating the LCA material and channel design, in concert with the reactive material characteristics, such that the transfer of shear stresses from the casing walls to the energetic filler provides control of reaction initiation and energy release characteristics. Coupling of the resulting chemical and kinetic energies will provide tunable performance, enabling control of reactivity and sensitivity of the energetic material. The rate of energy release in reactive powder mixtures is limited by the rates of mass transport; thus design of cell wall geometry will be critical in facilitating controlled mechanochemical reaction initiation conditions and attaining maximized energy density.

10:40 AM Break

10:55 AM Invited

The Observation of Phase Changes in Metal Alloys under Irradiation: *Stuart Maloy*[1]; [1]Los Alamos National Laboratory

The extreme environment of irradiation and its effects on core materials is a central problem to the lifetime of these materials in the core of a reactor. This environment encompasses irradiation to doses greater than 200 dpa at temperatures from 400-600C. Materials undergo many changes under this extreme environment including embrittlement from agglomeration of defects, phase transformations, radiation induced segregation and helium embrittlement. Observations of phase changes include, dissolution of strengthening phases, precipitation of embrittling phases and amorphization of precipitates. In this talk, many examples of such observed phase changes will be discussed from previous studies at LANL in connection with plans for future work in these areas.

11:30 AM

Irradiation Damage on Iron-Related Defects Using Molecular Dynamics: *Hyejin Jung*[1]; S. Oh[1]; [1]NFRI

Reduced Activation Ferritic Martenstic Steels (RAFMS) is one of the prime industrial candidates for next fusion reactor. For several decades, impressive experiments on RAFMS have been conducted but not under the irradiation condition. A parallel attempt has to be required to obtain the material properties under this extreme environment using theoretical modelling and computer simulation. In this study, we review the influence of fusion environment on the nucleation of various point defects, these defect diffusions and local stress around the atomic cascade as changing Primary Knock-on Atom (PKA) Energy values and temperatures in pure Fe and in Fe-Cr alloy. The configurations of voids, Self-Interstitial Atoms (SIA) and stress fields which affect material swelling effect are dynamically investigated using Parallel Molecular Dynamics modelling. Furthermore, the irradiation effects in vicinity on the grain boundary are additionally examined in poly-Fe.

11:50 AM

Microstructural Evolutions during Very High Temperature Transients in Ni-Based Single Crystal Superalloys: *Jonathan Cormier*[1]; Michaël Arnoux[1]; Xavier Milhet[1]; Florence Hamon[1]; José Mendez[1]; [1]ENSMA/LMPM

During operating conditions, aircraft turbine blade can experiment a short and abrupt temperature increase due to engine failure (One Engine Inoperative ratings). To mimic these conditions, a specific burner rig, enabling heating and cooling rates close to 60-80°C/s between 1050 and 1200°C, was used to characterize high and very high temperature evolutions of the γ'-phase of Ni-based single crystal superalloys. A great impact of the heating and cooling rates on the mechanical properties is observed. γ' phase dissolution, precipitation and coalescence processes in relation with both the dislocation activity and the local chemistry are responsible for the observed creep behavior under isothermal and non-isothermal conditions. Therefore, both the γ'-phase area fraction and morphology can be used as a local temperature/stress probe. Interaction between the precipitates evolutions and the deformation mechanism will be especially highlighted.

12:10 PM

Resistive Properties of the Shape Memory Alloy AuZn under an Applied High Magnetic Field: *Alyssa Maich*[1]; [1]Los Alamos National Laboratory

AuZn undergoes a shape memory transition that varies with composition. Shape memory alloys are applied in many aspects of society today; from stents, in the biomedical field, to temperatures switches, orthodontic arch wires, and sunglass frames. AuZn is an excellent candidate for studying electronic properties of martensitic transformations because of the high degree of order in the system and extremely low transition temperature. Both single and polycrystalline samples of AuZn at various compositions were tested in a superconductive magnet and subjected to magnetic fields from 0-15T. A change in magneto resistance from negative to positive, on either side of the martensitic transition, was found in the 48%Au single crystal sample. The 48%Au polycrystalline sample showed history dependence with magnetic cycling.

12:30 PM Concluding Comments

POSTERS

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 Organizers: Mark Palmer, Kettering University; Christina Raabe, TMS

Mon AM-Wed PM — Room: 2nd/3rd Floor Foyers
February 16-18, 2009 — Location: Moscone West Convention Center

3-D FEM Simulation and a Physics Model of Thermal Proximity Effect of Phase-Change Random Access Memory: *Ke Sun*[1]; [1]University of California, Los Angeles

Thermal proximity effect of phase-change random access memory (PcRAM) is studied by 3-D finite element simulation. Results show that there is no essential worsening of thermal proximity issue as the device feature size scales down to ultra small dimension. A physics model has been developed to explain the underlying physics of this phenomenon and demonstrates that, to the first order approximation, the profile of temperature distribution will be scaled together with the device dimension.

3-D Finite Element Simulation of a Phase-Change Random Access Memory Cell with a Novel Self-Insulated Structure: *Ke Sun*[1]; [1]University of California, Los Angeles

In this work, we proposed a phase-change random access memory (PCRAM) cell with a novel self-insulated structure (SIS), which is expected to have better thermal efficiency than the conventional structures. 3-D finite element simulation is used to study the most power consuming RESET process for both SIS and conventional normal bottom contact (NBC) cells driven by a MOSFET. Instead of programming current, power consumption is investigated to give a more fundamental comparison between the two structures. Thermal proximity effect for both kinds of cells is directly analyzed by simulating a 3×3 device array. The potential slow-quenching issue of SIS is also discussed.

A Description of an Urgent Pot Cut out and Restarting Process at Alcoa Pocos: Roberta Camilli[1]; *Flávio Silva*[1]; Andre Abreu[1]; [1]Alcoa Alumínio S.A.

Through January 2008 the Brazil's energy scenario was critical impacting the prices involved. Due this, Alcoa Pocos de Caldas Smelter Team has done a significant effort to cut out and restarted 15 pots out of 288 pots in a short period of time. This paper will describe how these pots were effectively restarted in this short period of time. This description will detail: the procedure elaborated to cut out 15 pots in 3 days without delayed tapping and stubbing operation; the process control adjustments to minimize the lost of current efficiency at neighborhood pots; and the potlining activities in order to re-use cathodes from old pots successfully.

A Linear Multiple-Degree-of-Freedom Ultrasonic Motor Using Bi2O3 and Fe2O3 Co-Doped PMN-PZT Piezoelectric Ceramics: *Ying Yang*[1]; Qian Li[1]; Jiamei Jin[1]; [1]Nanjing University Aeronautics and Astronautics

A linear multiple-degree-of-freedom ultrasonic motor was fabricatd using Bi2O3 and Fe2O3 co-doped PMN-PZT piezoelectric ceramics. The electrial driving properties of the motor were investigated. It is found that the motor has large output force, easy to miniaturize. Because of the designd symmetrical position of piezoelectric ceramics, the motor has the advantage of fabrication simplicity. A combination of Bi2O3 and Fe2O3 was selected as a flux to sinter 0.375Pb (Mg1/3Nb2/3)O3-0.625Pb(Zr0.4Ti0.6)O3 ceramics at low temperature condition (lower than 1000°). The piezoelectric properties were determined as well according to the IEEE standard. It is justified that the Bi2O3 and Fe2O3 co-doping is very effective on the low temperature sintering of piezoelectric ceramics without degrading their performance.

A Research Study on the High Strength API Steel

Production for Sour Gas Pipelines: *Shahrokh Pourmostadam*[1]; [1]Mobarakeh Steel Company

With regard to the achievement of the latest global Technologies for Pipe transportation of natural gas, containing substantial amounts of H2S (sour gas) is becoming increasingly common. Transportation of sour gas through HSLA pipelines can lead to failure from two mechanisms, hydrogen induced cracking (HIC) and sulfide stress corrosion cracking (SSCC). Over the years, suitable measures in alloy design, steelmaking technology and downstream processing has resulted in sour gas resistant linepipe steels. To ensure better weldability, steels are today designed with lower carbon and carbon equivalent levels. The strength is derived through controlled rolling, resulting in a fine ferrite grain size. Grain refinement is the only strengthening mechanism which increases the strength and toughness properties concurrently.

AC Induced Corrosion of 13 Cr Super Martensitic Line Pipe Steel in Seawater: *Jenny Collins*[1]; David Olson[1]; [1]Colorado School of Mines

Alternating current (AC) corrosion in buried pipelines has been reported in the literature; especially common is the influence of overhead transmission power lines inducing current in the pipe. The mechanism of AC corrosion, however, remains not fully characterized and described. A number of possible AC corrosion mechanistic models are being considered and tested. These models will be presented. Isolation of the physical phenomena is being achieved through laboratory testing. Emphasis is centered on assessing the change in susceptibility to localized corrosion with and without high AC current densities. Pitting and environmental cracking, including hydrogen assisted cracking, are also being analyzed. Impedance probe measurements are being used to assess for extra-induced stirring in the near electrolyte region of the stainless steel. Asymmetry of AC current due to a difference in anodic and cathodic behavior at the metal-environment interface is also being explored as a possible cause of a potential self-bias, resulting in accelerated anodic and/or cathodic (hydrogen ingress) behavior, and will be described. Preliminary laboratory results to date have shown pitting in seawater of a 13 Cr Super Martensitic Stainless Steel pipeline sample under an AC current density of 3800 A/m2 after ten days, while a specimen in seawater under no applied AC had no evidence of pitting after 17 days. Furthermore, initial results show that seawater pH increased by 0.23, from 8.17 to 8.40 after testing with an applied AC, which is preliminary evidence in support of an AC corrosion model involving alkalization of the environment. Data and correlations of a full battery of tests will be presented and mechanistic interpretations will be given.

Addition of Nitrogen and Nickel in the Fusion Zone of Plasma Transferred arc Weldments in UNS 32760 Super Duplex Stainless Steel: Effect on the Microstructure and on the Pitting Corrosion Resistance: *Kostas Migiakis*[1]; George Papadimitriou[1]; [1]National Technical University of Athens

Super duplex stainless steels present excellent combination of strength and corrosion resistance due to their strict composition control and ferrite-austenite phase balance. This microstructural balance in the fusion zone and the HAZ of the weldments is often disturbed because of the rapid cooling rates. These changes in microstructure lead to the loss of the good corrosion and mechanical properties of duplex steels. The scope of this work is to study the effect of nitrogen addition in the plasma operation gases and the addition of higher nickel content in the filler metal, on the microstructure and pitting corrosion resistance of super duplex stainless steels welded by the plasma transferred arc technique. Results have shown that nitrogen addition in the plasma operation gases and higher nickel content in the filler metal has positive effects on the phase balance and the pitting corrosion resistance of the weldments.

Al-Based Complex Metallic Alloys: *Jean-Marie Dubois*[1]; [1]Institut Jean Lamour

Complex Metallic Alloys (CMA) comprise a broad family of crystalline compounds most often made of aluminum alloyed with transition metals, rare earths or metalloids, and characterized by huge crystal unit cells containing tens, when not hundreds, of atoms. As a result, properties are different, often surprisingly, from the properties of the pure constituents. An example is given by the low thermal, and electronic, conductivity of the icosahedral Al-Fe-Cu compound.The talk will pay special attention to the selection mechanisms of such complex phases forming from metals that form especially simple crystal architectures when pure. Resulting properties will be reviewed as well as potential applications, such as e.g. preparation of composites, thermal barriers, catalists, etc. The effort going on in Europe on such complex intermetallics in the frame of the FP6 Network of Excellence called CMA will be illustrated.

AlB_2 Particle Segregation in Al-Cu-Mg Composites by Means of Centrifugal Casting: *Hermes Calderón*[1]; Giovanni Sandoval[1]; Carla Príncipe[1]; O. Marcelo Suárez[1]; [1]University of Puerto Rico

In certain applications, a gradual variation of mechanical properties throughout a mechanical part is required. For example, gear teeth need a good wear resistance on and near the surface as well as a ductile core. In aluminum

matrix composites (AMCs) this is achieved by increasing the volume fraction of hard particles at the surface with respect to inner regions or core. The goal of this work has been to obtain functionally-graded AMCs inducing particle volume fraction variation through the matrix. The particle segregation occurs by centrifugal forces acting on denser AlB_2 dispersoids. To control the process several variables have been taken into account: Melt pouring temperature, mold temperature, centrifugal force (via rotation speed), solidification rate, volume fraction of particles and particle density. Adjusting the variables, complete AlB_2 particle segregation at the surface can be obtained in an Al-Cu-Mg matrix. The procedure can be used to fabricate specimens for flexural tests.

An Investigation on Growth Mechanism of Nano-Boric Acid Structures: *Mehmet Isik*[1]; Servet Timur[1]; [1]Istanbul Technical University

Nano-boric acid is being used in traditional lubrication oils due to providing low friction coefficient while it is friendly to environment. Also, recently it is shown that it improves motor performance when used in diesel fuels. In this study, growth mechanism of nano-boric structures were investigated and characterized by SEM and XRD. In the first stage bamboo shaped hollow structures (length: 25 µm, diameter: 1 µm, wall thickness less than 10 nm) are formed. By boric acid transfer in time, hexagonal like head (diameter: 5 µm, wall thickness: 25 nm) emerges and the shape becomes like a tadpole. After that growing occurs in 3-D and hexagonal head grows in bowl form, with nucleation of new particles (d: 10 nm) inside. Finally bowl-shaped structures are closed and coalesced.

Analysis of Boron Distribution in Low Carbon Steel by Neutron Autoradiography: *Dong Jun Mun*[1]; Kyung Chul Cho[1]; Eun Joo Shin[2]; Yang Mo Koo[1]; [1]Pohang University of Science and Technology; [2]Korea Atomic Energy Research Institute

It is well known that a very small amount of boron in steel is hard to be detected with electron spectroscopy because of its low atomic value, so that a delicate and special technique is necessary to observe boron distribution in steel. So, in this present study, characteristics of boron distribution with variation of cooling rate after austenitization were investigated in low carbon steel employing Neutron Autoradiography method. The composition of the steel used in this study are 0.042C-0.059Si-0.530Mn-0.016P-0.013S-0.028Al-0.040Mo-with 23ppm of B. The technique applied was based on the detection of 1.53MeV alpha-particles from the thermal neutron $10B(n,\alpha)7Li$ reaction. It was observed that, when samples are fast cooled(20°/s) from 1350° to holding temperature, boron are mainly segregated along grain boundaries. However, when samples are slow cooled(1°/s) from 1350° to holding temperature, boron are uniformly distributed over the whole specimen without segregated regions along grain boundaries.

Analysis of Dendritic Growth in Casting Alloys A356 with Cu and Modified with Sr, by: Optical Microscopy, Poles Figures and Thermal Analysis: *Francisco Esteves-Alcazar*[1]; Alejandro Garcia-Hinojosa[1]; Aline Hernandez-Garcia[1]; [1]Univ Nacional Autonoma De Mexico

One factor that defines the properties of a metal such as aluminium is the plane or direction of growth, because this is done anisotropy. In the case of the A356 alloy (Al-7Si-0.3Mg) in casting conditions this presents a dendritic morphology with precipitates of Si (eutectic) in acicular or plaques forms, which influence in conjunction with the grain size properties end of the alloy. The matrix will be very important as it is the largest fraction of the microstructure, so in the case of a piece of casting if not done a check on growth unidirectional, submit a piece growth in many directions, with some preference toward extraction of heat direction. But not only the eutectic Si determines the direction of preferential growth, it is also important the presence of alloying elements as well as the modification of silicon eutectic caused the addition of Sr.

Analysis of Mechanical Properties of Low Carbon Hot Rolled Steel with Composition and Process Parameters: Neural Networks Approach: *N. S. Reddy*[1]; Jae Sang Lee[1]; [1]Alternative Technology Lab

An artificial neural network (ANN) model is developed for the analysis and simulation of the correlation between the mechanical properties of low alloy steels and composition and processing temperatures. The input parameters of the model consist of alloy composition and process parameters. The outputs of the ANN model include property parameters namely ultimate tensile strength, yield strength, and percentage elongation. Good performance of the ANN model is achieved. The model can be used to calculate properties of low alloy steels as a function of alloy composition and process parameters. The individual and the combined influence of inputs on properties of low alloys steels is simulated using the model. The results are in agreement with experimental knowledge. Explanation of the calculated results from the metallurgical point of view is attempted. The developed model can be used as a guide for further alloy development.

AUMUND Cooling Conveyor for Hot Bath Material: Christian Niedzwiedz[1]; *Frank Reddemann*[1]; [1]AUMUND Foerdertechnik GmbH

The AUMUND company supplies equipment for raw material handling in cement, iron and steel as well as in primary aluminium industry. In these industries, the handling of hot and abrasive bulk materials demands tailor-made solutions of the conveying technique. For primary aluminium industry AUMUND has designed a cooling conveyor for defined cooling of hot bath material. The bath material will be charged out of pots into a crusher, make SMV, which will feed the cooling conveyor. Subsequently, the bath material will cool down from 850°C to below 300°C or 100°C. The outlet temperature will depend on the following process. HF gases will not be emitted into the environment by application of a special cooling hood connected to the existing dry scrubbing system. The cooling conveyor is operating successfully in several European smelters. The biggest of them will be installed in the UAE in the near future.

Bridgman Growth and Characterization of Ga1-XNixSb Crystal: A Magnetic Semiconductor: *Sushanta Kamilla*[1]; B.K. Samantaay[2]; S. Basu[2]; [1]Institute of Technical Education and Research; [2]Indian Institute of Technology

The present work, high purity Ga, Ni and Sb in required proportions were vacuum sealed in quartz ampoule and melted inside a vertical Bridgman furnace with well defined temperature profile. Subsequent pulling by a low speed motor produced ingots of 3 cm length and 0.7 cm diameter. The formation of Ga1-xNixSb ternary alloys with different concentrations of Ni was confirmed by XRD, a linear lattice parameter–composition relation, as postulated by Vegard's Law. The electrical properties of the grown sample were studied at different temperatures from 78K to 300K by Hall Effect measurements using van der Pauw configurations. The positive sign of Hall coefficient confirmed p-type conductivity. The magnetoresistance studies at different magnetic fields (<10kG) and in the temperature range 78K to 300K showed positive magnetoresistance and indicate low Curie temperature (<78K), which was confirmed by AC susceptibility study.

Carbon-Metal Composite Foams for Increased Catalytic Activity, Electron Transfer, and Heat Recovery: *Ben Poquette*[1]; Stephen Kampe[2]; [1]Keystone Materials LLC; [2]Virginia Tech

In the late 90's, a novel technique for fabricating high conductivity graphite foam was developed by Oak Ridge National Lab. With its unique properties, this foam has shown promise to revolutionize the performance of many commercial and defense related systems not limited to: high surface area electrodes, catalysts supports, useful heat recovery. Until recently, difficulties in joining graphite foam to other materials have hindered its incorporation into current platforms. A technique was developed, through cooperation with ORNL and Virginia Tech, which allows a strongly adhered, uniform metallic coating to be applied throughout the thickness of graphite foam. These metal coatings should serve to both solve existing short-falls (brittleness, lack of joinability, etc.) as well as lend their properties (magnetic, catalytic, solderability, etc.) to graphitic foam.

Characteristics of Friction Stir Welding on 6061-T6 Al Alloy for Upper Structure of Leisure Ship: *Kim Seong-jong*[1]; Jang Seok-Ki[1]; Kim Jong-Shin[1]; Lee Seung-Jun[1]; [1]Mokpo Maritime University

Recently, there has been a new appreciation of aluminum alloys as materials that are capable of reducing the environment load. Therefore, this study investigated the on characteristics in friction stir welded condition of 6061-T6 alloy for leisure ship. In friction stir welded by using probe diameter of 5mm for 6061-T6 with various traveling speed at the rotation speed conditions of 210 ~ 1800 RPM and 220~720mm/min., the best characteristics presented in traveling speed of 507mm/min and rotation speed 1100RPM. The maximum tensile strength and yield strength increased with the increasing of traveling speed. This research was financially supported by MOCIE and KOTEF through the Human Resource Training Project for Regional Innovation.

Characteristics of MIG Welding by ROBOT on 6061-T6 Al Alloy for Upper Structure of Leisure Ship: *Kim Seong-jong*[1]; Jang Seok-Ki[1]; Han Min-Su[1]; Park Jae-Cheul[1]; [1]Mokpo Maritime University

If aluminum were used as a substitute for FRP in ships, the result would be more environmentally friendly vessels that are easy to recycle. This study investigated the on characteristics in welded by ROBOT for 6061-T6 alloy with

the factor of welding materials. The hardness of heat affected zone is lower than those of welding and base metal. At the result of tensile test, the specimen welded with ER5183 presented excellent property compared with ER5556. The corrosion current density in base metal is the lowest value more than those of two welding materials. Acknowledge; This research was financially supported by MOCIE and KOTEF through the Human Resource Training Project for Regional Innovation.

Characterization Microstructural and Corrosion Performance Heat Treated in a New Al-Mg-Zn Alloy by: Optic Microscopy, SEM, Corrosion Test and Microstructural Predictions Using Thermocalc: Aline Hernandez-Garcia[1]; Bernardo Campillo-Illanes[1]; Edgar Onofre[1]; *Francisco Esteves-Alcazar*[1]; Sergio Serna[1]; Socorro Valdez[1]; [1]National Autonomus University of Mexico

All over the world the aluminum alloys applications has been increased over the last decade, principally due to its weight/strength ratio in aircraft and transport industry. The Al-Mg-Zn alloys has been used as sacrificial anodes for cathodic protection, in the present work the characterization of two new Al-Mg-Zn alloys, with modification on Mg and Zn contents, were performed. Several heat treatments were carried to modify the foundry microstructure. Corrosion tests and metallographic quantification of phases were performed, to find the sample with best heat treatment condition suitable for be an option to be used as anode sacrifice. Additionally we conducted a prediction of stable phases using Thermocalc software and comparing with experimental quantification.

Characterization of Heat Treatment of Aging Applied to a Steel API X-52, Aged at Different Times, by SEM, Optical Microscopy, Prediction and Analysis by Thermocalc: Adair Jimenez-Nieto[1]; Bernardo Campillo-Illanes[1]; Aline Hernandez-Garcia[1]; *Francisco Esteves-Alcazar*[1]; Sergio Serna[1]; [1]National Autonomus University of Mexico

It is important to be able to characterize and to consider optimal times of heat treatments for steel, API-X52 that in the last 50 years has increased significantly their use in the industry, mainly for pipes. The process of manufacture of these pipes diminishes their mechanical properties, reason why a study of several times of treatment sets out to be able to have one more an ampler vision of what it would be adapted to use. Two alloys of the serie API-X52 would be used for this study, the X52-E and the X-52PS, to which it analyzed its mechanical properties, their microstructure by means of optical microscopy, SEM and prediction of phases by the software Thermocalc.

Characterization of Microstructure, Mechanical Properties and Corrosion Resistance of Welded Joints of 2205 Duplex Stainless Steel: *Yefeng Bao*[1]; Xuco Song[2]; Ruhong Zhang[3]; Yun Zhou[4]; [1]Hohai University; [2]Provincial Key Laboratory of Advanced Welding Technology of Jiangsu University of Science and Technology; [3]United Offshore Construction Co. CONHW; [4]China Office of SAF

2205 stainless steel pipes were welded by flux-cored arc welding (FCAW) and shielded metal arc welding (SMAW). The microstructures and the ratio of phase of the base metal, heat affected zone (HAZ) and weld metal were examined by optical microscopy. The mechanical properties in the variable zones were also determined. Corrosion properties were evaluated by cyclic voltammetry and polarization tests in 3.5% NaCl solution. The results showed that the weld microstructures were ferrite/austenite duplex structure. The hardness of the filler passes of both two welded joints was lower than that of the root passes for the effect of the welding heat cycle. The toughness of SMAW joint was higher than the FCAW joint due to the high austenite content. The two welding joints had the similar corrosion mechanism, but the FCAW joint had better corrosion resistance than SMAW joint, as it present an adequate ferrite:austenite proportion.

Characterization of Oxides in Low-Carbon GMAW Weld Deposits for High Speed Applications: *Germán León*[1]; Jorge Acevedo Dávila[1]; Mauricio Garza[1]; Mario Trejo[1]; [1]COMIMSA

GMAW equipment is one of the most widely applied for automatic and semiautomatic processes due to the high speed that can be achieved. Trend is to generate high speed deposits with high heat inputs, taking care of weld penetration. Purpose of this work is to verify decrease of the mechanical properties of the weld deposits made under these conditions. In order to accomplish this purpose test coupons were made at different speeds with constant heat input to evaluate weld penetration by the characterization of present oxides. Results show that the amount of oxides increase with speed and microstructure changed. A neural network approach is done to determine critical speed for oxides growth.

Characterization of the NiAl-xFe2-xO4 Catalyst Obtained by the Combustion Reaction: *Lucianna Vieira*[1]; Patrícia Tatiana Santos[1]; Ruth Kiminami[2]; Heloysa Andrade[3]; Ana Cristina Costa[1]; [1]University Federal of Campina Grande; [2]University Federal of São Carlos; [3]University Federal of Bahia

The water–gas shift reaction (WGSR) is one of the key steps involved in the automobile exhaust processes, converting CO with water to hydrogen and carbon dioxide and including the produced hydrogen as a very effective catalyst for NOx removal. The objective of this work is synthesized and characterizes NiAlxFe2-xO4 catalyst by combustion reaction used urea as fuel. To synthesis used a vitreous silica crucible on a hot plate at 480°C. The resulting powders were characterized by XRD, FTIR, adsorption of nitrogen for BET and catalytic measures. The results show that the catalyst presents crystalline phase of inverse spinel and trace of NiO and two stretching bands below 1000cm-1. NiAlxFe2-xO4 with x = 0, 0.5, 1, 1.5 e 2 moles Al3+, presented value of superficial area 25; 31; 28; 41; 88 m2/g, respectively. The catalyst with x = 1.5 presented CO/CO2 conversion major of 91% and activity of 49.5 mmolg-1.h-1.

Chemical Species Quantification and Oxide Film Measurements of Metal Surfaces by X-Ray Photoelectron Spectroscopy (XPS): *Mark Biesinger*[1]; L.W.M. Lau[1]; A. Gerson[1]; R.St.C. Smart[1]; [1]University of South Australia / University of Western Ontario

Improvements in X-ray photoelectron spectroscopy (XPS) technology and data processing procedures have allowed for significant improvements in our ability to quantify the oxide and hydroxide structures on the surface of metals. Significant progress in the analysis of the transition metals, which are complicated by a number of spectral phenomena, has been achieved. As well, calculations allowing for a more precise measurement of passive oxide/hydroxide thicknesses have been developed and improved upon, particularly for Al, Fe and Ni species. Examples from a range of metal surfaces will be shown.

Combined Experimental-Numerical Approach to Study the Diffusion and Dissolution of Al2O3 in CaO-Al2O3-SiO2 Liquid: *Frederik Verhaeghe*[1]; Muxing Guo[1]; Junhu Liu[1]; Bart Blanpain[1]; Patrick Wollants[1]; [1]Katholieke Universiteit Leuven

Dissolution phenomena and, more generally, interactions between solids and fluids are ubiquitous in materials science and engineering. In this work we focus on the dissolution behavior of solid Al2O3 in CaO-Al2O3-SiO2 liquids, a system with applications in metallurgy, e.g., for the removal of inclusions, the addition of fluxes, and the degradation behavior of refractory materials. We compare experimental observations using confocal scanning laser microscopy with numerical simulations to analyse the dissolution behavior, leading to the identification of a diffusion-controlled dissolution mechanism and an estimation of the effective diffusion coefficient of Al2O3 and its activation energy in this system.

Comparison between Theoretically Predicted and Experimentally Observed Microstructures in Alloys from Nb-W-Cr System: *Krista Amato*[1]; Benedict Portillo[1]; Julieta Ventura[1]; Shailendra Varma[1]; [1]University of Texas at El Paso

The experimentally observed microstructures of Nb-20W-5Cr and Nb-20W-10Cr, wt.%, alloys have been compared with theoretically obtained isotherms from the Nb-W-Cr phase diagram. The isotherms were obtained from a commercially available Pandat™ program and are based on the recent thermodynamic data from the literature. The predicted microstructures for these alloys based on the calculated isotherms from this source and Metals Handbook are different. The microstructural dependence on the oxidation behavior of the two alloys in a range of temperature from 700 to 1400° C will be presented.

Comparison of Short and Long Crack Growth for Titanium and Aluminum Alloys: *Bernd Oberwinkler*[1]; Christian Oberwinkler[1]; Wilfried Eichlseder[1]; [1]University of Leoben

To estimate the lifetime of flawed components with the aid of fracture mechanics it's essential to know the crack growth behavior. Therefore the crack propagation has been characterized for short and long cracks in two different light metals, namely Ti-6Al-4V and AlSi9Cu3, respectively. The measurement of long crack propagation has been done on single-edge-bending specimens via potential drop method to determine the crack length. To investigate the short crack growth plane tension/compression specimens have been provided with initial cracks. The growth of the crack has been observed with a high resolution camera. The results of these experiments provide a basis for a correlation with S/N-curves, determined with specimens from high pressure die casts and forgings.

They include casting inhomogeneities (AlSi9Cu3) and surface flaws (Ti-6Al-4V) respectively which act as initial cracks.

Composites of Polyamide6/Ferrite for Absorbers of Electromagnetic Radiation: *Daniella Bezerra*[1]; Keila Machado de Medeiros[1]; [1]UFCG

Composite consists of a mixture or combination of the two or more, micro or macro constituents that differ in shape and chemical composition and, in essence, are insoluble in one another. The polyamide is a polymer that presents dimensional stability, good resistance to impact without notch and excellent chemical resistance. Already the ferrites are absorbers of electromagnetic radiation and have versatility to be used as a composite of ferrites. The composite of polyamide6/ferrite was obtained by mixing 10, 20, 30% of ferrite added to polyamide6 in a blender internal Haake. The objective of this work was to develop composites of polyamide6/ferrite to achieve superior properties or better in some aspects regarding the properties of each of its components. The results were very promising, with a good interaction between the ferrite and polyamide6, to be used as absorbers of electromagnetic radiation.

Computer Aided Design for Metal Strip Coil Shape Corrector Machine: *Mohamed Elsalmawy*[1]; M Mokhtar[2]; A Wifi[2]; [1]Kandil Steel Complex; [2]Faculty of Engineering, Cairo University

This thesis presents a new approach to the selection and design of metal strip coil shape correcting machine. Coil defects as well as coil properties are categorized and relevant required machines, namely, levelers, straighteners or flatteners are specified. These approaches are fed to a specially devised computer technique in order to calculate the required power for leveling process, the number of rolls, rolls dimensions and configurations. For a given fully specified machine specifications, a decision could be taken to either to purchase or to construct the machine. In case, the decision is to purchase; the computer program introduces steps for selection out of data base of machine suppliers. On the other hand, in case, it's decided to design a new machine, the computer program has been so arranged to coupe with this decision and the full design is achieved. The design procedure has been herein explained.

Constitutive Parameter Determination Using Instrumentation and Simulation of Electromagnetic Ring Expansion Experiment: *Anupam Vivek*[1]; Glenn Daehn[1]; Jason Johnson[1]; Yuan Zhang[1]; Geoff Taber[1]; Pierre L'Elpattenier[2]; Gregg Fenton[3]; [1]Ohio State University; [2]LSTC; [3]Applied Research Associates

The modeling problem of electromagnetic forming is often dominated by inertial acceleration by a magnetic field which is a much better posed problem than the traditional ones that are dominated by complex 3-D constitutive behavior and frictional effects. However, important aspects of the problem are dominated by the constitutive properties of the material, and often electromagnetic forming is performed in a high-strain-rate regime where reliable material strength data is scarce. Also, there is little or no data in cases where temperature rises significantly over very short times (tens of micro-seconds). This rapid temperature rise is very important to the material response because the short time scales largely preclude the material from recovery and recrystallization processes. This presentation will show how advanced instrumentation, particularly the *Photon Doppler Velocimeter (PDV)* can be coupled with electromagnetic ring expansion and provide avenues to characterize material and to critically validate numerical models of electromagnetic forming.

Conventional Windmills Integrated with Generator Based on Magnetically Augmented Rotational System: Nuggehalli Ravindra[1]; *Rohit Chauhan*[1]; Gaurav Devrani[1]; Fiorella Fuentes[1]; Tony Chow[1]; Howard Helfgott[1]; [1]New Jersey Institute of Technology

A normal approach for the design and implementation of magnetic engine for potential power generation is described .The engine comprises a flywheel that is driven by utilization of a large number of magnetic field sources. Wind power is considered to be a promising and encouraging alternative for power generation because of its tremendous environmental and social benefits, together with public support and government incentives. The wind, however, is variable, site specific and an intermittent source of energy. The application for this magnetic engine for variety of pollution free power generating schemes is described.

Corrosion and Mechanical Properties of Electro Plasma Deposited Zn-Ni Coatings: *Pratheesh George*[1]; Edward Daigle[1]; Danila Ryabkov[1]; [1]CAP Technologies LLC

Electro Plasma Technology (EPT) is a hybrid technology which employs plasma process in an aqueous electrolytic cell for cleaning, coating and surface modification of metals. Coatings can be deposited at a very high rate of 1 µm per second using environmentally friendly chemicals and has unique characteristics to it such as nano sized grains which imparts excellent corrosion resistance and mechanical properties. The salt fog testing under ASTM B117 specification and wet/dry cycle testing of Zn-Ni coatings deposited using this technology has shown excellent resistance against corrosion. The process fundamentals, microstructural characteristics and corrosion test results of coatings deposited using EPT will be presented. Hydrogen Embrittlement and Fatigue tests have confirmed the superior nature of these coatings and these results will be also discussed. These properties make it an excellent replacement choice for cadmium and hexavalent chromium based coatings.

Crystallization Kinetics and Thermal Stability of Amorphous Cu50Zr50 Alloy: *Ilkay Kalay*[1]; Yunus Kalay[1]; Matthew Kramer[1]; Ralph Napolitano[1]; [1]Ames Laboratory / Iowa State University

The Cu-Zr binary system is well known to have a wide composition range of glass forming ability, but yet a complex devitrification behavior. In the present study, the crystallization kinetics and thermal stability of the Cu50Zr50 amorphous alloys were investigated using a combined study of differential scanning calorimetry (DSC), in-situ high energy X-ray diffraction (HEXRD) and transmission electron microscopy (TEM) in isochronal and isothermal annealing conditions. The amorphous Cu50Zr50 alloy was found to devitrify into the orthorhombic Cu10Zr7, tetragonal Zr2Cu (C11b) and cubic CuZr (B2) phases simultaneously. The results from TEM at different stages of crystallization accompanied with calorimetry analysis will be presented to discuss the mechanism of crystallization kinetics in amorphous Cu50Zr50.

Crystallization of a Marginal Glass Forming Alloy with DSC and Kinetic Analysis: *Charley Yeager*[1]; Yunus Kalay[2]; Scott Chumbley[2]; Iver Anderson[2]; [1]University of Rolla; [2]Ames Laboratory of DOE/Iowa State University

A kinetic analysis was done for the crystallization of the marginal glass former AlSm10at%. Undercooling yields an amorphous bulk phase with quenched-in fcc Al nano-crystals at a density of 10^22 /m. Ribbons melt spun at 30 m/sec wheel speed were isothermally crystallized using DSC. TEM analysis was performed at different stages of crystallization to validate kinetic analysis results. Two simultaneous thermal events are seen in DSC due to crystallizations of the quenched in fcc Al and the primitive-cubic intermetallic. To analyze these separate events a deconvolution was performed on the DSC trace taken at 178 °C. JMA kinetics were used to approximate these events as well as other models. JMA kinetics describe the fcc event well for site saturated nucleation and interface controlled growth. The cubic event was modeled best with steady state nucleation and interface controlled growth. Peak deconvolution was viable, supported by kinetic analysis and TEM observation agreement.

Density Measurement of Hugoniot End States in Polycrystalline Materials Using Dynamic X-Ray Diffraction: *D. Milathianaki*[1]; J. Hawreliak[1]; B. S. El-Dasher[1]; J. M. McNaney[1]; T. Ditmire[2]; H. E. Lorenzana[1]; [1]Lawrence Livermore National Laboratory; [2]University of Texas at Austin

Measuring material density under extreme conditions of pressure and temperature induced by shock waves is important in identifying the state of the compressed solid and potential phase transformations such as melt. In addition, knowledge of density together with a shock wave parameter such as particle velocity can provide information on the material equation-of-state. We present an x-ray diffraction technique that has yielded promising results in the density determination of polycrystalline materials of a wide Z range. Specifically, we report on the density measurement of shock compressed states in polycrystalline Cu along with particle velocity measurement using velocimetry (VISAR). The potential of this technique in absolute equation of state determination is discussed. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Design and Application of Variable Contact Roll Contour on Backup Roll of Finishing Stand at a Hot Strip Mill: *Xiaodong Wang*[1]; Quan Yang[2]; Fei Li[1]; Ming Li[3]; Wei Yu[3]; Bin Li[3]; Baohui Zhang[3]; [1]Research Institute of Techonolgy, Shougang Steel Corporation; [2]National Engineering Research Center for Advanced Rolling Technology, University of Science and Technology Beijing; [3]Qian'an Iron and Steel Company of Shougang Steel Corporation

Hot strip rolling has a feature of severe and complex working condition. There are many disturbing factors affecting strip shape control, and all of them can be expressed concentratedly to be rolling force fluctuation and roll contour change during hot rolling process. VCR backup roll, with a contour curve of

six order polynomial expression, was designed and applied on a hot strip mill of Shougang Corporation to reduce the influences of rolling force fluctuation and roll shape change on strip shape control for improving the shape control performance. This kind contour curve of backup roll can make the contact length between backup roll and work roll adapt with the width of strip rolled under the function of rolling force, eliminate or reduce the adverse contact areas between rolls, enhance the cross rigidity of loaded roll gap and then increase the shape control performance of hot strip mill.

Design of Experiment to Minimize Fluoride and Particulate Emissions at Alumar: *Eliezer Batista*[1]; Nilton Nagem[1]; Valerio Gomes[1]; Edson Montoro[1]; Paulo Miotto[1]; Luicano Souza[1]; [1]Alcoa

Most of Aluminum plants have been minimizing the fluoride and particulate emissions at the main source, which is the pot rooms, in order to reduce the environmental impacts. Many actions and studies are in place currently at Alumar. A quantitative study was done to map and determine the impact of each operation in the fugitive fluoride emissions (HF) in the pot rooms. Then, this full factorial experiment 2k was run in order to identify the main factors and their impacts on fluoride and particulate emissions. The statistical model is showing that the fluoride emission has been affected mainly by pot draft, pot dressing, and usage of compressed air for housekeeping with R2 at 82%. Based on the models, it was recommended some actions which will minimize both of these emissions. In addition, this paper describes, step by step, how this kind of experiment can be applied in the Aluminum industry.

Determination of Strain Field and Inhomogeneity in Radial Forging of Tube Using FEM and Microhardness Test: *Mehdi Sanjari*[1]; Saeed Tamimi[2]; Ali Taheri[1]; [1]Sharif University; [2]Tehran Polytechnic University

Utilizing the FEM, the strain field in the radial forging process of tube is calculated at different process conditions and compared with the experimental results achieved using the microhardness test. The effect of various process parameters such as friction, axial feed, back push and front pull forces and die angles on the strain field are investigated. Using the results of the analysis, it is shown that the deformation inhomogeneity, introduced by an Inhomogeneity Factor (IF), is the highest in the internal surface of tube, while the maximum and minimum effective strains are appeared at the internal surface of tube and about the core of the tube thickness, respectively.

Development of Nanocomposites Based on Polyamide 6 and Polyethylene Blends: Pankaj Agrawal[1]; André Rodrigues[1]; *Edcleide Araújo*[1]; Tomás Mélo[1]; [1]Universidade Federal de Campina Grande

In this work, Nanocomposites based on Polyamide 6 (PA6) and Low Density Polyethylene (LDPE) blends were developed using organically modified clay(organoclay). EMA-GMA terpolymer was used as compatibilizer. The nanocomposites were prepared in an intensive batch mixer Rheomix 600 attached to a HAAKE System 90 torque rheometer equipped with roller blades, at 50rpm and 240°C for 15 minutes under air atmosphere. Initially, a Masterbatch containing 50 % (wt) of organoclay and 50% (wt) of LDPE was prepared. The mixing time was 10 minutes. Afterwards the following compositions were prepared: PA6/LDPE; PA6/LDPE/Organoclay, PA6/LDPE/EMA-GMA, and PA6/LDPE/Oganoclay/EMA-GMA. The degree of dispersion of the clay in the polymer (PA6 or LDPE) was evaluated through X-Ray Diffraction (XRD). The results showed that the clay was dispersed and exfoliated predominantly in the PA6 phase.

Development of Revabratory Furnace in Egyption Copper Works (ECW) by Using Reformed Natural Gas: *Mohamed A.Kawy Hammad*[1]; [1]Central Metallurgical Research and Development Institute

In ECW, revabratory furnace which used for smelting of scrape of copper and residual ands and cathodes from the next stages which carried out in copper after casting from this furnace .In this time, deoxidation process carrying out by wood as a resource of reduction gases such carbon monoxide, hydrogen and methane. That is the problem, using of wood causes the following: 1- Pollution of medium of copper melting (forming soot of smock above furnace); 2-low efficiency in removal of oxygen from copper and more contamination in copper matta causes in rising of heat to remove of it and increasing in cost and time of casing of copper; 3-high expencincive this problem was solved by using of reformed natural gas as a source of reduction gases (CO+ H2), this led to the following.

Effect of Coating Thickness on the Structure and Properties of C_f/2024 Alloy Composites: *Linli Wu*[1]; Guangchun Yao[1]; [1]School of Material and Metallurgy, Northeastern University

Carbon fiber surface metallization is designed to increase the wettability between carbon fiber and aluminum alloy matrix, but at the same time, coating thickness will affect the structure and properties of composite materials. Thick coating will change the components of the matrix alloy and change the performance of the base alloy. Otherwise, thin coating will not achieve the role of connections. In this paper, different thickness of the nickel-plated carbon fiber was selected to reinforce alloy 2024. The microstructure and mechanical properties of the composite materials was studied to determine the more appropriate thickness of the layer nickel plating. When the coating thickness was 0.7μm, carbon fiber and matrix alloy had a better interface, the mechanical properties of composite materials also was the best.

Effect of Cooling Rate on Linear Contraction Rate and Hot Cracking Trend of T10 Steel: *Zhijun Li*[1]; Quanzhi Sun[1]; Zhengqi Xu[1]; Honggang Zhong[1]; Jianping Liang[1]; Qijie Zhai[1]; [1]Materials Science & Engineering, Shanghai University

The effects of cooling rate ranging from 6°C/s to 1°C/s on the linear contraction and hot cracking of T10 steel are investigated. The results show that, on one hand, the linear contraction rate of T10 steel can hardly vary with the cooling rate decreasing. On the other hand, the cooling rate influences the hot cracking trend of T10 steel. The hot cracking always appears in the surface of T10 steel sample when the cooling rate decreases from 6°C/s to 2°C/s. However, as 1°C/s of cooling rate, there isn't the hot cracking in the surface of T10 steel sample. Meanwhile, the hot cracking force increases with the cooling rate decreasing, which means to the decrease in the hot cracking trend of T10 steel.

Effect of Deposition Conditions on the Optical and Chemical Properties of Sio_2 Films: *Xiaoyan Xu*[1]; Sergey Nikishin[1]; Vladimir Kuryatkov[1]; Ayrton Bernussi[1]; [1]Texas Tech University

Thin SiO_2 films were deposited by plasma enhanced chemical vapor deposition (PECVD) in N_2O/SiH_4 plasma. The influences of chamber pressure, substrate temperature, and RF power on growth rate, refractive index (RI), and etching rate of SiO_2 films are investigated. When the thickness of film increases from 21.8 nm to 88.5 nm the RI increases from 1.273 to 1.463 corresponding to the RI of bulk SiO_2. P-etch (15 HF:10 HNO_3:300 H_2O) experiments performed on these films show a decreasing etching rate with increasing film thickness, indicating that films with a lower RI also have a lower density and more pores. From the temperature dependence of SiO_2 growth rate the apparent activation energy of 600 cal/mol was estimated for the surface reactions. The species and pathways of the surface reactions as well as the effect of He and Ar plasma dilution on PECVD are also discussed.

Effect of Heat Treatment on Two New IGT Superalloys: *James Staley*[1]; Chuck Biondo[1]; [1]Alstom/PSM

Industrial gas turbine (IGT) engine buckets are made from creep and elevated temperature tensile and fatigue resistant investment cast nickel-based superalloys. Superalloys with improved mechanical properties can increase efficiency and lower emissions and engine life cycle costs. Power Systems Mfg, LLC (PSM), a subsidiary of Alstom Power Inc., has developed two new, proprietary superalloys, which exhibit higher mechanical properties than some current IGT superalloys. Specimens were solution heat treated at different temperatures followed by precipitation heat treatment. Heat treated specimens were tensile, low cycle fatigue and stress rupture tested. Properties to date showed a significant increase when the solution heat treatment temperature was increased to above the gamma prime solutioning temperature. The highest solution heat treatment temperature conducted so far rendered the highest mechanical properties. It is expected that even higher solution heat treatment temperatures below the eutectic melting temperature would result in higher properties.

Effect of Nitrogen Contents on Stacking Fault Energy in TWIP Steel Using TEM: *Tae-Young Ahn*[1]; Sung-Il Baik[1]; Yeon-Seung Jung[2]; Young-Kook Lee[2]; Young-Woon Kim[1]; [1]Seoul National University; [2]Yonsei University

Twin-induced plasticity (TWIP)-aided steel is widely studied as a next-generation structural materials because of its exceptional plasticity and high strength. Stacking fault energy (SFE) is known as the key parameter to control the deformation and strengthening of high-Mn TWIP steel. Nitrogen was incorporated in the Mn-TWIP steel to reduce the Mn content and the change of SFE was measured with the content of nitrogen. SFE values were obtained in

TEM by measuring the curvature of direct extended 3-fold node of dislocation network. As Mn contents was reduced from 18 to 15 wt% , SFE was changed from 34.5 to 13.9 mJ/m2. When nitrogen was added, however, SFE increased up to 17.4 mJ/m2 with 0.09wt% of nitrogen in the alloy. It was confirmed from the X-ray diffraction that the addition of the nitrogen in the Fe-15Mn TWIP steel alloy suppressed the formation of the ε-hcp phase.

Effect of Probe Shape with Traveling Speed in Friction Stir Processing for 5456-H116 Al Alloy: *Kim Seong-jong*[1]; Park Jong-Seek[1]; Han Min-Su[1]; Park Jae-Cheul[1]; [1]Mokpo Maritime University

This paper investigated friction stir processing with probe traveling speed to improve mechanical characteristics. From result of experiment with probe screw, the case of existence of probe screw considers that has good material characteristics because of by plastic flow by heat which comes from high friction heat. In full screw probe, the material characteristics decrease with traveling speed increase and the best characteristics is 15 mm/min. It was shown the best characteristic when experimental conditions are 800 RPM, 15 mm/min. And then this case has hardness, which advancing side is higher than retreating side and heat-material effected zone has the lowest one. Acknowledge: This research was financially supported by MOCIE and KOTEF through the Human Resource Training Project for Regional Innovation.

Effect of Residual Sodium Contents on the Structure and Morphology of Titanate Nanotubes for Hydrogen Storage: *Bora Lee*[1]; Sun Jae Kim[2]; Chang Hee Lee[1]; Kyung Sub Lee[1]; [1]Hanyang University; [2]Sejong University

The titanate nanotubes synthesized by hydrothermal method using rutile powder in NaOH solution usually show a small amounts of sodium in the structure. In this work, the sodium contents have been controlled by changing the pH levels in the washing condition. The three samples with different contents of residual sodium were prepared and fired from 200°C to 800°C. Under relatively higher pH, the titanate nanotubes without annealing had the structure of A2Ti2O5•H2O (A=Na or H), the shape remained tubular upto 400°C and finally converted to Na2Ti6O13 of rod-like shape at 800°C. However, the sample at a lower pH (no residual sodium) was converted to anatase in the granular form at 400°C. The rod-like shape absorbed a relatively higher capacity than the tubular shape. The relationship between the hydrogen storage, the structure and morphology of nano titanate was discussed.

Effect of the Addition of Two Alkaline Activators on the Hydraulic Behavior of Composites Cements with Ground Granulated Blast Furnace Slag, Fly Ash and Geothermal Waste: *Javier Lozano*[1]; Lauren Gómez-Zamorano[2]; [1]IPN-ESIQIE, Programa de Maestría en Ciencias en Ingeniería Metalúrgica; [2]Universidad Autónoma de Nuevo León, Facultad de Ingeniería Mecánica y Eléctrica, Programa Doctoral de Ingeniería de Materiales

The mechanical properties and the hydraulic behavior of environmentally friendly cement pastes of ground granulated blast furnace slag (GGBFS) - fly ash (FA) - geothermal waste (GW) and Portland cement (PC) were investigated. The replacement materials were activated with 1, 4 and 7% of Na2O using NaOH and water glass. The pastes were cured up to 90 days at 20°C. The results indicated that the mechanical properties were improved with the activator load and with the use of water glass; nevertheless the latter reduced the workability of the pastes. The FA addition reduced the properties but increased the workability of the pastes. Moreover the increase on GGBFS and GW load enhanced the compressive strength and the formation of hydration products as analyzed by SEM and an important consumption of clinker phases and calcium hydroxide were also found by XRD, indicating a contribution of the replacement materials on the hydration reactions.

Effect of the Matrix Viscosity on the Morphology and Mechanical Properties of Polypropylene /Brazilian Organoclay Nanocomposites: André Rodrigues[1]; Tomás Melo[1]; *Edcleide Araujo*[1]; Pankaj Agrawal[1]; [1]Universidade Federal de Campina Grande

In this work, the effect of Polypropylene (PP)viscosity and the Brazilian organically modified clay (organoclay) on the morphology and the mechanical properties of PP/Organoclay Nanocomposites was investigated. The nanocomposites were prepared using a co-rotating twin screw extruder. Two grades of PP with different viscosities were used as a matrix and PP-g-MA was used as a compatibilizer. The nanocomposites were characterized by X-Ray Diffraction (XRD), Transmission Electron Microscopy (TEM) and Mechanical Properties. XRD results showed that a predominantly intercalated nanocomposites were formed. The nanocomposites formation was not affected by the PP viscosity. These results were confirmed by TEM. Mechanical properties results showed that the elastic modulus and the tensile strength were improved.

Effect of Thermo-Mechanical Processes on Alloy 909 Stress-Rupture Properties: *Octavio Covarrubias*[1]; Osvaldo Elizarraras[1]; [1]Frisa Aerospace

Alloy 909 is a Ni-Fe-Co alloy which properties make it useful for gas turbines and rocket-engine applications. Several turbine-engine components, like casings, seals and others can be made from this alloy by ring-rolling processes. This alloy is a precipitation hardenable material which properties are result of forging procedures and heat-treatment processes. As most materials processed for industrial purposes, components made of this alloy shall be mechanically and microstructurally tested to validate promoted properties: stress-rupture is a key characteristic to be evaluated. From an industrial standpoint, this job summarizes the effects on stress-rupture properties when several alloy 909 forgings are produced according to different ring-rolling and heat-treatment variables. Experimentation results are complemented by light microscopy and SEM evaluations, allowing determination of production parameters to promote best alloy properties. It must be mentioned, since implementation of proposed production parameters, no deviation due to metallurgical causes was reported.

Effects of a Tantalum Addition on the Morphological and Compositional Evolution of a Model Ni-Al-Cr Superalloy: *Christopher Booth-Morrison*[1]; David Seidman[1]; [1]Northwestern University

The effect of a 2.0 at.% addition of Ta to a model Ni-Al-Cr superalloy aged at 1073 K is assessed using scanning electron microscopy and atom-probe tomography. The addition of Ta is found to result in appreciable strengthening, and the morphology is found to evolve from a bimodal distribution of spheroidal precipitates, to cuboidal precipitates aligned along the elastically soft <001>-type directions. Tantalum is observed to partition preferentially to the γ'-precipitate phase and suppresses the mobility of Ni in the γ-matrix sufficiently to cause an accumulation of Ni on the γ-matrix side of the γ'-precipitate/γ-matrix heterophase interface.

Effects of V and C Additions on the Mechanical Properties of High Strength Invar Base Alloy: Ae-Cheon Yun[1]; Jin-Hwa Song[2]; Tae-Kwon Ha[3]; *Kee-Ahn Lee*[1]; [1]Andong National University; [2]RIST; [3]Kangnung National University

The Fe-Ni based Invar alloys usually have relatively low strength and hardness. This study sought to examine the effect of V & C additions on the mechanical properties of the high strength invar type alloy. By using the FactSage program for thermodynamic equilibrium phase simulation, base alloy represents the Mo2C carbide can be formed as main precipitate. V2 alloy (V+C additions) indicated to appear Mo2C+(V,Mo)C carbides. It was apparent in mechanical results that the vanadium carbide can improve hardness and strengths of high strength invar type alloy. The tensile fractography of V2 alloy represented ductile transgranular fracture mode and voids were initiated between the vanadium carbide particle and matrix. Superior properties of high strength and low CTE could be obtained by (V,Mo)C precipitation in the V2 alloy. By examining appropriate condition for cold rolling and heat treatment, the high strength of 1.556GPa could be successfully obtained in V2 alloy.

Elastic Moduli and Mechanical Properties of Some Bulk Metallic Glasses: John Plummer[1]; I. Todd[1]; I. A. Figueroa[1]; R. J. Hand[1]; H. A. Davies[1]; [1]University of Sheffield

The relationships between the elastic moduli and response to deformation of bulk metallic glasses were investigated. Five bulk metallic glasses were prepared from high purity elements via suction casting. The results confirm that there exists a correlation between energy absorbed to failure during compression testing and the bulk to shear modulus ratio. This finding is developed such that it corresponds only to the elastic component of energy absorption, and so is not capable of predicting extensive plasticity. Instead, the ideas of the shoving model are applied to plastic deformation, identifying new criteria for the relationship between shear and bulk moduli and plasticity. This idea is subsequently tied into the widely considered apparent dependency of free volume to plastic flow. The importance of structural features frozen in during the glass transition is therefore isolated meaning that it is suitable to consider the effect of glass fragility. Therefore, it may be possible to specify different criteria to maximise elastic and plastic energy absorption separately, opening new possibilities with regard to engineering the mechanical response of bulk metallic glasses.

Electrochemistry Study on Epoxy Resin to Anti-Corrosion Performance of Reinforced Bar in the Concrete: *Daowu Yang*[1]; Chengfeng Wang[1]; Zhongliang Xiao[1]; [1]Changsha University of Science and Techonology

Corrosion behavior of reinforced bar in concrete was studied by simulating the 4×4 array wire-beam electrode in this paper. These reinforced concretes have been coated respectively in different ways: blank, iron wire with coating resin in surface, concrete with coating resin in surface, concrete and iron wire with coating resin. By measuring open-circuit potential of iron wire, the impact of different ways of coating were studied on the corrosion of concrete. The result showed that it is the best protection way to coat resin on the surface of concrete, which keep the open-circuit potential within the passivation range all the time, so as to ensure the integrity of the passivation membrane.

Evaluated of the Structure and Morphology of the NiAl2O4 Catalysts Obtained by Combustion Reaction Using Glycine as Fuel: *Lucianna Vieira*[1]; Ana Cristina Costa[1]; Elvia Leal[1]; Normanda Freitas[1]; Hélio Lira[1]; [1]University Federal of Campina Grande

NiAl2O4 is an oxide well known by its great thermal stability and chemical inertia, for this reason, is very used as catalysts, catalysts support and optical layers. The synthesis of these catalysts is based on combustion reaction using the thermodynamic concepts from propellants chemical. The aim of this work is to evaluate the influence of the glycine fuel when it was used in the stoichiometric proportion and with the excess of 10% and 20% in the preparation of NiAl2O4 by combustion reaction. The powders were characterized by DRX, nitrogen adsorption for BET, granulometric distribution, and infrared spectroscopy. The results show the presence of NiAl2O4 as major phase and traces of NiO and Ni for all studied powders. The size of the crystallites was 22, 17 and 9 nm to the stoichiometric composition, 10% and 20% in excess of glycine, respectively. The powders presented morphology with agglomerates of irregular plates shape.

Evaluation of Characteristics in Slow Strain Rate Test for Solution Heat Treated Al-Mg Alloy: *Kim Seong-jong*[1]; Han Min-Su[1]; Kim Jong-Shin[1]; Jang Seok-Ki[1]; [1]Mokpo Maritime University

The Al alloy specimen was carried out to prevent corrosion with solution heat treatment. The optimal heat treatment over the range from 10 to 240 min. involved heating specimens for 120 minutes at 420°C and then cooling them in water. The SSRT in sea water revealed that heat treatment under optimal conditions produced improved elongation, time-to-fracture and amount of dimples compared with the as-received specimen. The optimum cathodic protection range in slow strain rate test presented -1.4V~ -0.7V. The characteristics of stress corrosion cracking and hydrogen embrittlement by solution heat treatment at optimum condition are improved 10.20 and 9.51 percent, respectively. Acknowledge: This research was financially supported by MOCIE and KOTEF through the Human Resource Training Project for Regional Innovation.

Evaluation of Structural Strength in Body Structure of Container Freight Car: *Sung Cheol Yoon*[1]; [1]Korea Railroad Research Institute

This paper describes a carbody structural analysis and the result of its loading test. The purpose of this study is to evaluate the safety and functionality of the A carbody operating under maximum load. The freight car was designed with SM490YA steel and SM490Y steel for the railway transportation. The carbody of rolling stock is a principal structure supporting major equipment of underframe, and container freight. So, the strength evaluation of this structure is important and can be the core technique in rolling stock analysis. Both structural analysis and loading test were performed under the loading condition. Prior to the evaluation, finite element method software was used for structural analyses on stress distribution in a carbody of freight car. The strain gages were attached on the carbody based on the FEM results. The test results showed that the carbody is safe and stable under the condition of designed load.

Evaluation of Toughness Deterioration by an Electrochemical Method in an Isothermally-Aged N-Containing Austenitic Stainless Steel: Maribel Saucedo-Muñoz[1]; *Victor Lopez-Hirata*[1]; [1]Instituto Politecnico Nacional

This work shows the evaluation of the cryogenic toughness deterioration by means of an electrochemical method in a N-containing austenitic stainless steel aged at temperatures of 700, 800 and 900°C for times from 10 to 1000 minutes. The aging process at 700 and 800°C caused the decrease in the Charpy V-Notch impact energy at -196°C because of the intergranular precipitation of carbides. The scanning electron microscope fractographs of the Charpy V-Notch test specimens showed the presence of intergranular brittle fracture. The degree of sensitization was determined by the ratio of the maximum density current generated by the reactivation scan to that of the anodic scan, Ir/Ia using the double-loop electrochemical potentiokinetic reactivation test. The Charpy V-Notch impact energy decreased with the increase in the Ir/Ia ratio. This relation enables to estimate the deterioration of cryogenic toughness because of the thermal aging in this type of steel.

Evolution of the Microstructure of As-Rolled Ti-43Al-9V-Y Alloy with Different Heat Treatments: *Fantao Kong*[1]; Yuyong Chen[1]; [1]Harbin Institute of Technology

Microstructures developed in TiAl intermetallics sheet after heat treatments in the α, α+γ and α+ß regions of the Ti-Al phase diagram have been studied. The Ti-43Al-9V-Y alloy sheet material investigated had a starting microstructure consisting of equiaxed γ grains with a small volume fraction of B2 phase mainly located in γ grain boundaries. Samples were heat treated at different temperatures ranging from 1250°C up to 1320°C. After different heat treatment, the equiaxed γ grain size of the sheet does not increase dramatically but precipitation of B2 phase lamellas in equiaxed γ grains is observed upon furnace cooling. Furthermore, microstructure of Ti-43Al-9V-Y alloy sheet transferred from γ+B2 phase microstructure to DP microstructure after the heat treatment of 1300°/30min. The identification of the various phases present in the microstructures was made with the help of XRD, which also helped to understand the nature of the phase transformation in Ti-43Al-9V-Y alloy.

Evolution of Zn + NaCl Foams, Characterization and Interconnection in Open Cell: *Said Casolco*[1]; [1]Tecnológico de Monterrey

The structure and hardness of a Zn+ NaCl prepared with sintering process. It established parameters for the synthesis of metal foam with high porosity. The consolidation process consisted of the alloy powders mechanic of Zn and a foaming agent NaCl purity make to at room temperature, were conducted three different compositions that are: 80% Zn 20% NaCl, 60% Zn 40% NaCl and 50% Zn 50% NaCl. The mechanical properties were determined from trials of hardness and mechanical strength in a universal machine. It was determined that the best is the composition of 80% Zn 20% NaCl with a maximum load of 146 MPa. The energy absorption of 72% and a hardness of 50 HV0.5, The effect of Zn weight fraction are significant for different applications with potential use in the aerospace, automotive and biomedical applications.

Experimental Phase Studies in the TeO2 – WO3 System: *Ercin Ersundu*[1]; Miray Çelikbilek[1]; Günkut Karaduman[1]; Nuri Solak[1]; Suheyla Aydin[1]; [1]Istanbul Technical University

Tellurite glasses are of great importance in fiber optic amplifying applications and as laser hosts. Comparing with silicate, borate and phosphate glasses, tellurite glasses have superior properties, such as low-phonon energy, high refractive index, high dielectric constant, good corrosion resistance, thermal and chemical stability. TeO_2 is the main but the conditional glass former; therefore, addition of a secondary component, such as heavy metal oxides, increases the glass forming ability. The present study aims investigation of the phase equilibria in the TeO_2-WO_3 system. Three different compositions, (1-x) TeO_2 – x WO_3 (x = 0.10, 0.15, 0.20 in molar ratio) were prepared. The samples were heated in a platinum crucible for 30 minutes at 750°C, then were quenched and crushed. TG/DTA, XRD and SEM techniques were used to investigate the samples.

Exploring the 3D Nanospace of Defects Formed in Ni-Based Superalloys Using Atom-Probe Tomography, Electron Microscopy, and Dual-Beam Focused Ion-Beam Microscopy: *Yaron Amouyal*[1]; David Seidman[1]; [1]Northwestern University

Turbine blades utilized in aeronautical jet engines and land-based power generators are fabricated from single-crystal Ni-based superalloys, which offer superior strength and creep resistance at high temperatures. However, the formation of freckles as chains of misoriented grains along the solidification direction of the alloy results in the degradation of the blades. We employ atom probe tomography (APT) in combination with scanning and transmission electron micorscopies to investigate the microstructure and chemistry of freckles in multi component Ni-based alloys at all pertinent length scales. This powerful combination of techniques provides us with high detectability (< 10 at. ppm) analysis extending from the 10 nm to 10 mm length scales. Additionally, we apply site-specific measurements using the dual-beam focused ion-beam (FIB) microscope to lift-out samples for APT from specific regions of interest. Thus, we determine the roles played by different low-concentration (<500 at. ppm) alloying elements in the formation of freckles.

Fabrication and Characterization of Squeezed Cast Aluminum Matrix Composites with Boride Reinforcements: *Lilia Olaya-Luengas*[1]; Elvin Estremera[1]; O.M. Suárez[1]; [1]University of Puerto Rico

Aluminum-copper alloys reinforced with borides were successfully fabricated by a squeeze casting technique employing squeezing pressures from 0 to 100 MPa. The distribution of reinforcements on composite was determined and the effect of pressure on density and hardness of composites was established. Besides, the borides stability was analyzed while the composites were heat treated. The pressure responses in the composites squeezed were investigated by optical microscopy, Vickers microhardness testing, Thermal Differential Analysis (DTA) and X-Ray Diffraction (XRD) advanced techniques.

Failure Analysis in a Total Knee Prosthesis Metal-Polyethylene Implanted in an Active Patient: *Marco Hernandez-Rodriguez*[1]; Arturo Juarez-Hernandez[1]; Alan Castillo[1]; Jose Diabb[1]; Alberto Perez-Unzueta[1]; [1]UANL FIME

One of the most important problems with total joint prosthesis is the early wear. The present work is about a metal-polyethylene total knee prosthesis that failed in service prematurely within 5 months by severe wear in a 50 year old female active patient with natural bony misalignment in her legs. In order to determine the origin of the failure, the prosthesis components were analyzed by means of visual inspection, optical microscopy, scanning electronic microscope (SEM), energy dispersive spectroscopy (EDS), chemical analyses, roughness test, Fourier transformer infrared (FTIR), gel penetration chromatography (GPC) and differential scanning calorimeter (DSC). The studies showed that the failure was due to a degraded UHMWPE resulting in low mechanical and tribological properties, along with an unbalanced high stress by an uncorrected surgery collocation, lead an atypical accelerated wear failure.

Finite Element Model of Compression of a Polycrystalline Layer Showing Banding Behavior: *Ryan Quarfoth*[1]; Md. Zakaria Quadir[2]; Michael Ferry[2]; Lori Bassman[1]; [1]Harvey Mudd College; [2]University of New South Wales

Finite element models were developed for compression and rolling of metal sheet. The model uses experimentally-determined polycrystalline grain structures with orientation-dependent material properties. Specifically, anisotropic Young's modulus values are included and orientation-dependent yield stresses are calculated based on the Schmid factor with respect to the normal direction. The model shows bands of increased localized shear strain, and the geometry of the bands is a product of the grain structure. Areas of increased shear strain can lead to localized flow in the microstructures in the form of microbands and shear bands. Their inclination in the model at approximately 40 degrees relative to the rolling direction and initiation at the grain boundaries is consistent with experimental findings in conventionally rolled material and in layered aluminum-alloy structures.

Formation, Structure and Deformation Behavior of High Strength Ti-Based Alloys with Fe: *Dmitri Louzguine*[1]; Larissa V. Louzguina-Luzgina[1]; Akihisa Inoue[1]; [1]WPI Advanced Institute for Materials Research, Tohoku University

The high-strength metastable eutectic and hypereutectic Ti-Fe, Ti-Fe-Co, Ti-Fe-Cu, Ti-Fe-Co-Sn and Ti-Fe-Cu-Sn alloy ingots were produced by arc-melting. The structure of these Ti-based alloys containing about 20-40 at.% LTM (LTM-late transition metals, here Co or Cu) at high enough Fe/Co or Fe/Cu ratio (=1) is found to consist of the primary dendrites of an ordered cP2 intermetallic (IM) compound having a rounded dendritic morphology and an eutectic consisting of the cP2 IM compound and a disordered supersaturated cI2 ß-Ti solid solution. On compressive test at room temperature these Ti-based alloys exhibit a high ultimate mechanical strength values (some of them exceeding 2000 MPa) and a plastic deformation of 4-24%. The formation of a composite-like structure with a hard carcass of the IM phase in the relatively soft eutectic matrix enabled both high strength and ductility. The deformation behavior and the fractography of these Ti-based alloys were also studied.

Fundamental Study on the Diffusion of PbSn Eutectic Solder Electroplated on 95Pb5Sn High-Lead Solder: *Chun-Cheng Lin*[1]; Chih Chiang Chang[1]; C. Robert Kao[1]; [1]National Taiwan University

Many of the flip-chip solder joints were composed of the 95Pb5Sn solder bump, and the PbSn eutectic pre-solder. In order to understand the interfacial reaction behavior, 95Pb5Sn/37Pb63Sn diffusion couples were used. The diffusion couples was processed high temperature storage tests at various temperatures (100, 130, 150, and 175°C) for 100~2000 hrs. It is found that the grain growth in the initially fine eutectic PbSn microstructure is the key microstructural evolution during the interdiffusion.

Gas Injection System for Ion Beam Induced Deposition and Etching: *Andrew Madison*[1]; Donovan Leonard[1]; Anuj Dhawan[2]; Phillip Russell[2]; [1]Appalachian State University; [2]Duke University

The versatility of focused ion beam (FIB) nanofabrication has been well established for tasks such as TEM sample preparation and circuit or mask repair. We report the added capability of material deposition and etching, using ion beam induced chemistry, made possible by mating a commercial gas injection system (GIS) with a FIB. Deposition parameters relative to several organometallic gases including, C9H16Pt, (CO)6W, and gold precursor will be discussed in the context of the development of novel nanostructures. In exhibition of the enhanced capability realized with FIB/GIS, the fabrication of templates for bio-related plasmonic sensing will be presented. Experimental protocols for the nanofabrication of binary Pt/W metallic nanowires will be included along with variables for beam induced XeF2 etching of HfO2 thin films for microelectronic device cross section decoration.

Gas Sensing Properties of MoO3 Thin Film Deposited Using Chemical Vapor Transport of MoO3(OH)2: *Young Jung Lee*[1]; Young Moon Kim[1]; Han Seob Kim[1]; Dae-gun Kim[1]; Young Do Kim[1]; [1]Hanyang University

MoO3 thin film has strongly attracted attention as a conductance-type gas sensor because of high sensitivity to various gases such as NOx, CO, H2, and NH3 in the temperature range of 300-600°C. There are many deposition techniques for MoO3 film such as thermal evaporation, sputtering, chemical vapor deposition, and pulsed laser deposition. Characteristics of films are dominated by deposition technique and its parameters, so that a challenge of new approach is required as well as extensive studies of structural and physical properties to obtain enhanced sensing properties. In this study, a new fabrication technique of MoO3 film for a gas sensor is suggested. MoO2 film was deposited at 500°C in H2 by chemical vapor transport of MoO3(OH)2 during hydrogen reduction of MoO3 powder and the deposited film was annealed at 400°C in O2 to fabricate MoO3 phase. Gas sensing properties of the films were discussed relating with microstructural evaluations.

Growth of ß-Ga2O3 Nanowires and Nanobelts Prepared by Physical GaAs Evaporation: *Hee-Suk Chung*[1]; Seoung-Bum Son[1]; Tae Jun Ko[1]; Seul Cham Kim[1]; Do Hyun Kim[1]; Kyu Hwan Oh[1]; [1]Seoul National University

Nano-structured materials can perform unique optical, electronic, and structural properties as compared to their bulk forms on account of quantum confinement effects and a high fraction of chemically similar surface sites. One-dimensional (1D) nanostructures have drawn extensive attractions due to their distinguished properties resulting from their unique size and dimensionality. Among various 1D nanostructures, monoclinic(ß)-Ga2O3, a wide-band gap compound with a band gap of approximately 4.9eV at room temperature, is a promising transparent conductor for the coming generation of optoelectric devices in the deep-ultraviolet wavelength region. Recently, ß-Ga2O3 have been fabricated via arc discharge, laser ablation, powder evaporation, etc. However, little literature is only available with regard to understanding the vapour-liquid-solid via oxygen atmosphere on ß-Ga2O3 nanowires synthesis. In this letter, we report fabrication and characterization of ß-Ga2O3 nanowires synthesized through GaAs physical evaporation. As-synthesized nanowires were characterized with scanning electron microscopy, transmission electron microscopy, X-ray diffraction.

High-Pressure/High-Temperature Raman Studies on Thermal Storage Materials –Neopentylglycol (NPG): *Vamsi Krishna Kamisetty*[1]; Juan Carlos Fallas[1]; Wen-Ming Chien[1]; Dhanesh Chandra[1]; Erik Emmons[2]; Aaron Covington[1]; Raja Chellappa[3]; [1]University of Nevada, Reno; [2]U.S. Army Edgewood Chemical Biological Center; [3]Carnegie Institute of Washington

Pressure-Temperature phase diagrams for the materials neopentylglycol (NPG) were determined using high-pressure/high-temperature Raman scattering experiments. The presence of thermal transitions between orientational order and disorder in this material make it important and has been suggested for use as thermal storage materials. At room temperature there is no phase change observed upon increasing the pressure up to ~10 GPa, but at 0.5 GPa and above 50°C there is a orientational order/disorder transition in which NPG goes into γ-phase. Similar phase change into γ-phase is seen again at 1.16 GPa and above 126°C. Further Increasing the pressure to 2.08 GPa and at 151°C the order/disorder transition shows that NPG enters into a new γ-phase. Pressure-Temperature phase diagram of NPG has been determined based on the temperature-dependent and pressure-dependent Raman data acquired.

High-Temperature Microstructures of ZrB2-SiC Composites Prepared by Spark Plasma Sintering: *Ipek Akin*[1]; Filiz Sahin[1]; Onuralp Yucel[1]; Takashi Goto[2]; Gultekin Goller[1]; [1]Istanbul Technical University; [2]Tohoku University

In this study, ZrB2-SiC composites were produced using SPS at high temperatures, above 2100°C, and microstructural features were investigated. The temperature of the die increased at 0.8°C/s in vacuum under a pressure of 10 MPa. Pulsed direct current (60 ms/on, 10 ms/off) was applied during the SPS process. The temperature of the die was measured by an optical pyrometer and the shrinkage of the specimens was continuously monitored during the process. The microstructure of ZrB2-SiC composites containing 40 mass% SiC sintered at 2200°C consisted of irregular texture composed of ZrB2 and fine a-SiC grains in addition to the elongated a-SiC grains. For the ZrB2-80 mass% SiC composite, porous structure was detected. The decomposition of SiC may have caused the formation of large pores at higher temperatures, 2280°C, 2300°C and 2360°C.

High Pressure Raman and X-Ray Studies of Tris(Hydroxymethyl)Amino methane (TRIS): *Vamsi Krishna Kamisetty*[1]; Wen-Ming Chien[1]; Juan Carlos Fallas[1]; Dhanesh Chandra[1]; Erik Emmons[1]; Aaron Covington[1]; Raja Chellappa[1]; Simon Clark[1]; [1]University of Nevada, Reno

Organic thermal energy storage materials are useful for thermal energy storage due to the presence of solid-state phase transition where the latent heat can store energy. The effects of temperature and pressure on X-ray diffraction patterns and Raman spectra of tris(hydroxymethyl) aminomethane (TRIS) (C(CH2OH)3NH) were measured. DSC and in-situ X-ray diffraction results show the solid-state (α-orthorhombic to γ-BCC) phase transition of TRIS occurs at 133.7°C at ambient pressure (1 atm). At room temperature, high pressure synchrotron X-ray diffraction patterns and Raman spectra using Diamond Anvil Cell (DAC) show TRIS undergoes a phase transition (α to ß) at ~1 GPa. A new high pressure ß-phase was observed from ~1 GPa to 9.3 GPa. The effects of hydrogen bonding on the broad OH and sharp NH stretching modes will be discussed. Detail results of temperature dependent effects on high pressure Raman spectra and Pressure-Temperature (P-T) phase diagram of TRIS will be presented.

High Strength FeCo-Based Multiphase Composite Alloys with Good Magnetic Properties: *Ran Li*[1]; Mihai Stoica[1]; Gang Liu[1]; Jürgen Eckert[1]; [1]Leibniz-Institute of Solid State and Materials Research (IFW) Dresden

It is well known that near-equiatomic FeCo-based alloys offer exceptional magnetic properties. However, notorious brittleness of this alloy obstructs its industrial application. By controlling rapid-solidification condition and designing multicomponent alloying, we produced a family of FeCo-based multiphase composite alloys with good mechanical and magnetic properties. Comparing with equiatomic FeCo binary alloy, the "designing" alloys exhibit 3~4 times improvement of yield stress and obvious plastic deformation of 5~20% during compressive test. The structural analysis indicated that homogeneous fined grains, induced by the control of liquid solidification, and morphologic construction of multiphase composite, designed by the choice of alloying elements, endow these alloys with good mechanical properties. Furthermore, although the alloying decreased the saturation magnetization of resulting alloys, it still remains ~ 2 T as high as the result of pure iron. These FeCo-based multiphase composite alloys combining with advantages of structural materials and functional materials have a good potential application.

High Temperature Corrosion Behavior of Sputtered K38 Nanocrystalline Coating with Yttrium Additions in Molten Sulfate: *Fuhui Wang*[1]; Wen Wang[1]; Ping Yu[1]; [1]Institute of Metal Reserach, Chinese Academy of Sciences

A two-dimension nanostructured coating, which chemical composition is similar to the Ni-based substrate alloy, was deposited by sputtering technique. The influence of various amounts of yttrium addition on high temperature corrosion behavior of the sputtered coating in the presence of molten 75wt.%Na_2SO_4+25wt.%K_2SO_4 at 1173K was investigated. The results indicated that nanocrystallization for superalloys increased the corrosion resistance significantly through the rapid formation of continuous exclusive alumina scale. The addition of yttrium further improved the corrosion resistance of the nanocrystalline coating by increasing the stability of the alumina scale. The synergetic effects of nanocrystallization and yttrium addition on the high temperature corrosion behavior in molten sulfate were discussed.

High Temperature Oxidation of Steels in Air and Co2-O2 Atmosphere: *SangHwan Bak*[1]; DongBok Lee[1]; [1]Sungkyunkwan University

Three kinds of hot rolled steel slabs, viz. high strength steel, bake hardened steel and low carbon steel, were oxidized isothermally between 1100 and 1250°C for up to 2 hr in 1 atm of air and an 85%N2-10%CO2-5%O2 gas mixture. The steels oxidized in a similar fashion in both atmospheres. The oxidation process followed an initial linear rate law, which then gradually transformed to a nearly parabolic rate law. Thick, porous and nonadherent scales formed rapidly, due to the high oxidation temperature. The scales formed consisted of Fe2O3, (Fe2O3+Fe3O4), (Fe3O4+Fe2O3+FeO) and (FeO+Fe3O4) from the outer surface. The presence of supersaturated oxygen beneath the scale resulted in grain boundary oxidation and the formation of internal oxide precipitates.

Impact of the Brazing Process Variables in the Reduction of Porosity of Copper Alloys with Copper and Silver Filler Material: *Misael Hernández*[1]; Jorge Acevedo[1]; Mauricio Garza[1]; [1]Corporación Mexicana de Investigación en Materiales S.A. de C.V., Ciencia y Tecnología

In this study the relation between welding time, temperature and filler material variables were studied in copper tubes used in the freezing system and welded by brazing. The most important variables were the welding time and the cleaning treatment. The best result were found with 350°C and 11 seconds with cleaning treatment, reducing the porosity in the welding zone but the base material started to recrystallize. The result found at 350°Cand 7 seconds without cleaning treatment was more porosity.

Impression Creep of a Thermo-Stable PMR-15 Polyimide: *Rong Chen*[1]; Fuqian Yang[1]; Y. C. Lu[1]; G. P. Tandon[2]; G. A. Schoeppner[3]; [1]University of Kentucky; [2]University of Dayton Research Institute; [3]Air Force Research Laboratory/RXBC

Polyimides based on the polymerization of monomeric reactants (PMR) approach have the potential for high temperature applications in aircraft engines. The performance of the PMR-based structures depends on the mechanical durability of the PMR at high temperatures, such as creep and stress relaxation. In this work, the creep behavior of PMR-15 polyimide was studied, using the impression technique in the temperature range of 250 to 300ºC and the impression stress of 111 to 277 MPa. The impression stress corresponded to about 3.5 time of the compressive stress, i.e. 31.7 to 79.1 MPa. It was found that there existed a steady state creep for the creep tests with temperatures of 280ºC and higher, from which a constant impression velocity was calculated. The steady state impression velocity increased with temperature and the impression stress with a stress exponent of about 2.5.

Improvement of Tensile Ductility of Heavily Rolled and Recovery Annealed Aluminum Alloy Sheet: *Ni-Hsing Lee*[1]; Jyun-Hao Chen[1]; T. Tseng[2]; P. W. Kao[1]; [1]National Sun Yat-sen University; [2]China Steel Corporation

For non-heat treatable aluminum alloys, strength can be achieved by heavy cold working, but poor ductility is often accompanied. In order to restore some ductility, a low temperature recovery annealing may be applied, in which the annealing is carried out at a temperature below the onset of recrystallization. The recovery annealing often produces yield drop, which is followed by flow localization, early onset of necking, and poor ductility. In this work, Al-Fe-Mn alloy sheets produced by heavy cold rolling (>95%) followed by recovery annealing were investigated. Anisotropic tensile tests were carried out with stress axis along the directions of 0°, 45°, and 90° from rolling direction. It was observed that the presence of Mn in solid solution could improve both the tensile strength and ductility of the recovery annealed aluminum alloy sheet. Microscopic observations were also performed and related to the tensile properties.

Indentation Creep Properties of Self-Similar Indenters: S. V. Thube[1]; P. Kumar[1]; *A. Elmustafa*[2]; [1]Applied Research Center-Old Dominion University-Jefferson Laboratory; [2]Old Dominion University

Finite element analysis is used to simulate indentation creep experiments with variable indenter tips. Indentation creep simulations of self-similar indenters i.e., cone, pyramid, and berkovich are presented. The purpose of the analysis is to identify the relationship between the strain rate sensitivity of the hardness, v_H, and that of the flow stress, vσ in materials with variable elastic-plastic properties. The results from the pyramidal and berkovich indenter tips will be compared with results already published for a conical indenter tips to complete the set of analysis for self-similar indenters. Previously it was asserted that v_H differs from vσ, but the ratio v_H/ vσ is found to be a unique function of where H is the hardness and is the modulus relevant to Hertzian contact. Due to self-similarity, it is expected that this result will hold for the other two indenters tips (pyramidal and Berkovich).

Influence Local Use of Ageing Effects in Multiphase Steels for Designing Local Properties of Constructional Elements: *Heinz Palkowski*[1]; Mehdi Asadi[1]; [1]TU Clausthal

The investigations deal with processes leading to local effects of strengthening in multiphase steels, being characterized by good formability, continuous yielding, high strength and a strong bake hardening and ageing effect. Dual phase and complex phase steels are under investigation to examine the effect of thermo-mechanical processing parameters on local ageing ability. For this purpose local heat treatment by laser are studied, as well as stability of local ageing on the adjusted strength. The local heat treatment leads to an increase of hardness and strength and to local strengthening of the material. The stability of the local strengthening effect could be confirmed. Partial heat treatment of multiphase steels by laser can open a new field of application for the local use of the bake hardening effect. Chance is given to influence only relevant areas, thus representing a potential for energy-saving.

Influence of Additives on Immobilization Process of Heavy-Metal Containing Waste Residues Using Elemental Sulfur: *Liyuan Chai*[1]; Li Wang[1]; Xiaobo Min[1]; Yu Wu[1]; Yunyan Wang[1]; [1]Central South University

In this paper, three additives, namely sodium hydroxide, calcium hydroxide and sodium carbonate, were used to enhance the immobilization of cadmium and zinc in sulfuration neutralization sludge using elemental sulfur. The results showed that the pH of the leachate increased as the addition rate of these three additives increased. Both NaOH and Ca(OH)2 greatly improved the performance of immobilization. Na2CO3 also enhanced the immobilization of cadmium and zinc, however, to a less extent. After analyzing the products of metal oxides mixed with sulfur and additives or without any additive at 413K, the results revealed that metal sulfuration did not occur during the sulfur immobilization process without any additive. However, with the addition of NaOH, cadmium sulfide and zinc sulfide were produced. Other two additives could not promote metal sulfuration, while they enhanced the immobilization of cadmium and zinc simply by increasing the pH value of the leachate.

Influence of Heat Input on Microstructure and Mechanical Properties of Laser Beam Welded Superalloy Inconel 718: *Akin Odabasi*[1]; Necip Ünlü[1]; Gültekin Göller[1]; Niyazi Eruslu[1]; [1]Istanbul Technical University

The effect of heat input from laser beam welding (LBW) on the microstructral and mechanical properties of superalloy Inconel 718 were investigated. Four different heat input produced to evaluate the geometry of weld seams. Full penetration was achieved in all weld experiments. The analysis of optical and field emission scanning electron microscopy together with micro-hardness based on ISO 9015-2:2003(E) were performed. Increasing the amount of heat input from 74.5 J/mm through 126.5 J/mm changed the resulting weld shape from a wine glass shape to a stemless wine glass shape with wider surface bead widths. The effect of heat input was significantly clear at the widths of the mid- and upper-side of the weld seam. It was observed that the differences of the heat input affected the solidification rate. The secondary dendrite arm spacing increased with increasing heat input.

Influence of Processing Conditions on Development of PE/PE-g-MA/ Organoclay Nanocomposites: Luana Kojuch[1]; Renata Barbosa[1]; *Edcleide Araújo*[1]; Tomas Melo[1]; [1]Universidade Federal de Campina Grande

Nanocomposites developed with silicates in layers represent an alternative to the composites developed with conventional filler, because they use minimum levels of nanofiller. In this work, polyethylene/PE-g-MA/organoclay nanocomposites were produced in a Torque Rheometer Haake in these conditions: 190°C, 60 and 120rpm, for 7 and 14 minutes. The systems were characterized by X-ray diffraction (XRD). The obtained results indicated that the PE/PE-g-MA/ organoclay nanocomposites presented intercalated and/or partially exfoliated structures for the 120 rpm and 7 minutes, probably due to bigger number of intercalation of polyethylene molecules between the layers of the organoclay. For the time of 14 minutes, the material showed a little degradation probably due to excessive time in the mixer.

Influence of Submerged Tandem Arc Welding on HAZ Toughness of X80 Micro Alloy: *Sadegh Moeinifar*[1]; [1]Azad University

X80 HSLA steel is a high grade microalloy steel that is used for this research. Tandem SAW with two or excess electrode is an economic process for joining microalloy steels components. welding process is done with four wires but lowering in heat affected zone toughness for high grade microalloy steels. Toughness in heat affected zone (fusion line, coarse grain HAZ and fine grain HAZ) studied. Welding done in different amount of heat input. Microstructure and Impact energy with CVN (charpy V notch) studied in -50°C. Heat affected zone in microalloy steels is complex due to many phases (polygonal ferrite, quasi polygonal ferrite, widmanstatten ferrite, acicular ferrite, granular ferrite, bainite, M/A, inclusions). Impact energy changes with heat input up to optimum and increased about fifty percent. Microstructure study with SEM shown that M/A island,austenite grain growth and ferrite side plate is a major factor in CGHAZ toughness.

Interfacial Bonding Characteristics of Cu Thin Film on FR-4 Substrate for Chip-in-Substrate Applications: *Kyoung-Jin Min*[1]; Sung-Cheol Park[1]; Ki-Wook Lee[2]; Jae-Dong Kim[2]; Do-Geun Kim[3]; Gun-Hwan Lee[3]; Young-Bae Park[1]; [1]Andong National University; [2]Amkor Technology Korea Inc; [3]Korea Institute of Materials Science

Chip Embedding is increasingly adopted as future electronics technology due to its trend of high density and high performance. One responsible technology is to embedded active device into a dielectric substrate by build-up process, for example, chip in substrate (CiS) structure. This embedding of active devices technology needs Cu metallization of micro-via for contacts I/O pad on embedded chip with outer layers, however, the poor interfacial adhesion between Cu via and dielectric substrate can lead to limitation of interfacial reliability at actual using conditions. In this study, we investigated the effects of the ion-beam treatment conditions on chemical bonding of FR-4 substrate surface and also on the interfacial adhesion of Cu via to FR-4 systems in order to understand the interfacial bonding mechanism. Extensive interface analyses using FE-SEM, AFM and XPS were performed to understand the fundamental interfacial bonding mechanism and to find the optimum conditions of ion-beam treatment, respectively.

Investigation of Intermetallides, Obtained in Ti-Al System under Shock Wave Loadings: *Nikoloz Chikhradze*[1]; George Oniashvili[1]; Mikheil Chikhradze[1]; [1]Mining Institute of Georgia

The paper describes the results of investigations of the reactions in Ti-Al system induced on shock wave front developed during the chemical explosions. Experiments were conducted in the cylindrical and normal mode of shock-wave configuration. Theoretically calculated the energetic characteristics and stress tensor components in steel container containing the Ti-Al reaction mixture. The phase constitution of obtained samples, microstructure and mechanisms of intermetallides formation are investigated depending on the initial ratio of components in reaction mixture. Welding zone of intermetallides and cylindrical surface of steel ampoule were studied and determined the micro-hardness distribution in structure. The above mentioned and structure/properties relationships are discussed in the paper.

Investigation of the Influence of Silver and Tin on Trivalent Europium Ions in Aluminophosphate Glass: *José Jiménez*[1]; Sergiy Lysenko[1]; Huimin Liu[1]; Esteben Fachini[2]; Oscar Resto[2]; Carlos Cabrera[2]; [1]University of Puerto Rico at Mayagüez; [2]University of Puerto Rico at Río Piedras

The spectroscopic properties of Eu^{3+} ions in aluminophosphate glass containing silver and tin have been studied. Glasses were prepared by the melt-quenching technique in which Ag nanoparticles (NPs) were embedded upon heat treatment (HT), and studied by optical absorption, photoluminescence (PL) spectroscopy, X-ray photoelectron spectroscopy, and transmission electron microscopy. An enhanced Eu^{3+} ions emission was observed for non-resonant excitation near 270 nm. Optical measurements suggest that light absorption occurs at isolated Ag^{+} ions and/or twofold-coordinated Sn centers followed by energy transfer to Eu^{3+}. The PL properties and decay characteristics of silver, tin and europium in the host have been assessed in order to elucidate the nature of energy transfer. The effect of HT on Eu^{3+} ions is discussed along with likely Ag NP-Eu^{3+} interactions in the nanocomposite.

Joining of TiAl with Reactive Multilayer Thin Films and TiNi Thin Foils: *Sónia Simões*[1]; Filomena Viana[1]; Ana Ramos[2]; Maria Vieira[2]; Manuel Vieira[1]; [1]Faculdade de Engenharia, Universidade do Porto; [2]Faculdade de Ciências e Tecnologia, Universidade de Coimbra

TiAl application in aerospace components depends not only on the alloy design but also on the processing, surface modification and joining. In this work, we join gamma-TiAl with Ni/Al multilayer thin films; TiNi foils were used as a braze alloy to fill the bond gap. The multilayers were deposited into TiAl samples by d.c. magnetron sputtering with periods of 5, 14 and 30 nm. Joining experiments were performed under a pressure of 50 MPa at 800, 900 and 1000ºC

for 1 hour in a vertical furnace, with a vacuum level better than 10-4 mbar. The microstructure of the cross-sections of bond interface was analysed by energy dispersive X-ray spectroscopy (EDS) and characterized by scanning electron microscopy (SEM) and high resolution transmission electron microscopy (HRTEM). Sound joints are obtained with a combination of reactive multilayer thin films and TiNi thin foils. Several NiAlTi intermetallic compounds are formed in the interface region.

Large Cold Deformation Behavior of a High Strength Ti-Alloy: *Yongqing Zhao*[1]; Zhengping Xi[1]; [1]Northwest Institute for Nonferrous Metal Research

How to reduce the cost is one of the main research directions in the Ti field. Ti26 is a new high strength Ti alloy with tensile strength over 1250MPa developed by Northwest Institute for Nonferrous Metal Research. After large cold deformation, its yield strength increases quickly, its tensile strength and elongation also increases with the increase of deformation amount. The observations of microstructure show that the grains size is not well distribution and big grains are exist with not so large deformation, and the grains are fine with the increase of deformation amount. The evolution of its microstructure undergoes two processes, that is deformation and recrystallization, after large cold deformation and solution. After solution, its microstructure becomes equiaxed grains through recrystallization. The large cold deformation mechanism of Ti-26 alloy is twin and slip.

Laser-Co2 Process Optimization to Stainless Steels in the Manufacture of Control Emission System in the Automotive Application: Arturo Novales[1]; Arturo Reyes[1]; [1]Corporacion Mexicana De Invertigacion En Materiales

This paper shows the results to the investigation project to evaluate the impact of the variables of laser-CO2 process, apply in the manufacture of control emission system in the automotive industry. The impact of the energy power, velocity and shielding gas in the microstructure, tensile properties and micro-hardness was evaluated. The data had been treated to obtain a multivariate statistical model to the process optimization. The model was validated and it has been applying in the real process, increasing the productivity and use to other technological projects.

Latest State of Continuous Carbon Paste Preparation with Buss Kneader Technology: *Hans-Ulrich Siegenthaler*[1]; Joel Stampfli[1]; Peter Franz[1]; [1]Buss AG

The "Buss Kneader" is since over 50 years the leading technology of continuous anode paste mixing. The main obstacles of anode manufacturers today are the rising costs of pitch and coke, followed by their deteriorating quality. Intensified mixing process together with micro dispersion of the pitch is the answer to this dilemma. These specific process requirements have been analysed and converted to the latest generation of Buss Kneaders, having improved mixing performance. For this development Buss AG used the experiences of the recent year's development of the advanced Buss technology. A systematic process oriented approach was one of the key elements for reaching the ambitious goals. This paper will present the latest state of the developments to mix green carbon paste with specific focus on high production capacities and for achieving the processing and economic advantages as requested by the anode producers today and tomorrow.

Lorentz Force Flowmeter in Industrial Application: *Vitaly Minchenya*[1]; Christian Karcher[1]; Yuri Kolesnikov[1]; Andre Thess[1]; [1]Ilmenau University of Technology

Lorentz force velocimetry is an innovative technique for non-contact measurement of the flow rate and accumulated mass of moving conductive fluids like high-temperature liquid metal alloys. In this work we present the results of industrial tests of the Lorentz force flowmeter (LFF) in a secondary aluminum production plant. The measurements were carried out in an open channel within which the primary melt is transported from the rotary furnace to the holding furnace. The uncertainty of measurement is obtained by comparing the measured accumulated mass with the results of preliminary weighting of the alloy components.

Magnetic Properties and High Frequency Characteristics of FeCoZrO/ZrO2 Multilayered Thin Film: *Kai-Xin Liu*[1]; Jeng-Gong Duh[1]; [1]National Tsing Hua Univ

During last decade, the IT technology has offered huge application of soft magnetic films for high frequency devices, like power converters. Fe-Co alloy thin film exhibits very large saturation magnetization. Thin films with fine grains with size smaller than ferromagnetic exchange length and with multilayer structure lead to low coercivity. In this study, multilayered soft magnetic thin films of FeCoZrO/ZrO2 were deposited by DC reactive magnetron sputtering. Zr and O were added to refine the grain size and to increase the resistivity, respectively. The field annealing was followed by film deposition to release internal stress and to induce uniaxial anisotropy. The composition, the static magnetic properties and the complex permeability of films was determined by EPMA, VSM and permeameter, respectively. The resistivity was measured by conventional four-point method. The effect of multilayered structure and the addition of Zr and O on magnetic softness would be probed and discussed.

Manufacturing of Copper Foam by Electro-Deposition: *Jun Li*[1]; Qinghua Tian[1]; Ling Huang[1]; Xueyi Guo[1]; [1]Central South University

A novel method for preparing porous copper foam was proposed in which the polyurethane foam as substrate was processed by degreasing process, roughening process, conductive treatment and copper electrodeposition. Influence of different solution compositions and operation conditions on factors such as current efficiency and cell voltage was discussed. Optimum experiment conditions were got by optimizing the factors.

Mechanical and Microstructural Observations during Creep of Fine-Grained Ti-45Al-5Nb-0.2B-0.2C: *Dennis Peter*[1]; Gopal Babu Viswanathan[2]; Martin Wagner[1]; Gunther Eggeler[1]; [1]Ruhr University Bochum; [2]The Ohio State University

Constant load creep experiments were conducted on the hot-extruded Ti-45Al-5Nb-0.2B-0.2C (at.-%) alloy in the 700°C-800°C temperature range. The material exhibits a fine-grained duplex microstructure consisting of equiaxial γ grains of about 2.5 μm grain size, as well as lamellar α2/γ colonies. Microstructures before and after creep were analyzed using scanning electron microscopy (SEM), transmission electron microscopy (TEM), electron back scatter diffraction (EBSD) measurements, and a complementary specimen preparation technique with focused ion beams (FIB). TEM analysis after creep reveals that dislocation creep and some twin activity occurs in the lamellar colonies. In contrast, only few deformation substructures are found in the equiaxial grains. These results and surface observations of FIB tracer lines on specimens crept under high purity Argon atmosphere indicate that the equiaxial γ grains (representing 65-75 vol.-% of the material) may well deform by grain boundary sliding.

Mechanochemical Synthesis and Characterization of Titanium Diboride Powder: *Duygu Agaogullari*[1]; Fikret Aynibal[1]; Osman Cihan Demirhan[1]; Ismail Duman[1]; [1]Istanbul Technical University

Titanium diboride classified as advanced ceramic is commonly produced using high temperature technologies. In this study, TiB_2 powder was produced at room temperature by mechanochemical process providing magnesiothermic reduction of TiO_2 (anatase) and native anhydrous B_2O_3 which were employed in stoichiometric amount. Following the synthesis of TiB_2 in multi-axial ball mills in constant ball-to-powder weight ratio (10:1), the intermediate products will be refined by HCl leaching. In experimental studies, the parameters in milling and leaching which affect the microstructure of final product and the efficiency of process, such as milling type (Spex and Platenery ball mill), milling time (1-40 hours), PCA (% 2 stearic acid) and excess Mg (5%-20%) addition, leaching duration (from 3 minutes to 2 hours) and acid concentration (1M - 3M) will be examined. The intermediate and final products were characterized by Particle Analyzer, XRD, SEM/EDS and DTA analyses. Also, leaching solutions were analyzed by AAS.

Methane in Syngas Conversion over Ni/A-Al2O3/ ZnO Catalyst: *Lucianna Vieira*[1]; Laedna Neiva[1]; Heloysa Andrade[2]; Ruth Kiminami[3]; Ana Cristina Costa[1]; [1]University Federal of Campina Grande; [2]UFBA; [3]UFSCar

This work has as aim the development Ni catalyst supported in a-Al2O3/ZnO, to be applied in the reaction of steam reforming of the methane. The Al2O3/ZnO catalytic support was obtained by synthesis method of the combustion reaction. The catalytic support was characterized by X-ray diffraction, textural analysis by BET method, SEM and TEM. The support was submitted to impregnation with Ni by humid method. After of the impregnation the catalyst was characterized by adsorption/desorption of N2 for BET, XRD and submitted to catalytic test in laboratory. Al2O3/ZnO catalytic support presents crystalline structure and nanosize particles with crystallite size of 55 nm and similar morphologic aspect to of the α-Al2O3 pure. The Ni impregnations promoted an alteration textural in the structure porosity of the catalyst. The result of catalytic test showed that the

developed catalyst in this work is extremely efficient in the obtainment of the syngas from the methane.

Microstructure and Mechanical/Electrical Properties of Nanostructured High-Strength, High-Conductivity (HSHC) Cu Material: *Timothy Lin*[1]; Chunhu Tan[1]; Bob Liu[1]; [1]Aegis Technology Inc.

With continual size shrinking of microelectronic systems, the electrical wires, circuit leads, contacts, and interconnects in these systems are desired to possess both good electrical conductivity, and high mechanical strength. Commercially pure Cu is a traditional material of choice for these components, which however suffers the limitations of low mechanical strength. Recent investigations suggested that the formation of a special class of nanocrystalline microstructure would provide the opportunity to achieve both high strength and high conductivity (HSHC), in contrast with conventional nanocrystalline Cu materials generally featured with high strength and yet substantially reduced electrical conductivity. Aegis Technology has successfully demonstrated the fabrication of bulk HSHC Cu materials by using a cost-effective synthesis and consolidation process that can be scaled up for mass production. In this presentation, we will report the microstructure, mechanical/electrical properties and their correlations of this HSHC Cu material.

Microstructures and Mechanical Properties of Copper Alloyed Austempered Ductile Irons: *Usanee Kitkamthorn*[1]; Ittipon Diewwanit[2]; [1]Suranaree University of Technology; [2]Chulalongkorn University

Microstructures and mechanical properties of copper alloyed austempered ductile iron were investigated. The standard tensile specimens were austenitized at 900°C for 60 minute and then austempered at 300°C and 340°C for a range of 60-6000 seconds. Results showed that amounts of bainitic ferrite and retained austenite increase with increasing austempering time. The transformation of the higher content of copper alloyed iron shows significantly the difference of microstructure between eutectic cell and intercellular boundary. The yield strength and ultimate tensile strength and %elongation increase with an increase of austempering time. The mechanical properties of austempered ductile irons satisfied the high strength grade of standard ASTM A897M:1990 when austempering was carried out at 300°C. However, the austempering at 340°C can not produce the more ductile grade. The microstructure revealed that the amounts of bainitic ferrite, martensite and retained austenite are in good agreement with the tensile properties.

Microstructures of Electron Beam Melted (EBM) Biomaterial Ti-6Al-4V: *Adnan Safdar*[1]; Liu-Ying Wei[1]; [1]Malmö University

Ti-6Al-4V alloy is an attractive material to be considered as biomaterial. The current work evaluates the microstructures by SEM/EDX and optical microscopy of the solid and net-shape Ti-6Al-4V alloy produced by Electron Beam Melting (EBM). The microstructures are influenced by the cooling rate, processing parameters in EBM system and re-heating of the existing layer during the melting of subsequent layer. Layer structure and occasional columnar beta grains have been observed, with growing direction parallel to built direction. The interior of ß grains consists of alternating a / ß phases. The ß phase in the colonies resembles rod shape embedded in the plates. Along the ß grain boundaries more or less continuous a layers were observed. In comparison to solid samples uneven surfaces and pores were observed in the net shape structure. Microhardness evaluation of the EBM produced alloys were also carried out and compared with conventionally produced alloys.

Mixture of Calcium Hydrides and Lithium Borohydrides for Hydrogen Storage Materials: *Hongwei Yang*[1]; Andrew Goudy[1]; [1]Delaware St Univ

Destabilization of lithium borohydrides for reversible hydrogen storage materials has been studied by using calcium hydrides as a destabilizer. In our experimental work, mechanically milled mixtures of LiBH4 and CaH2 are shown to store about 13 wt% hydrogen. The equilibrium pressures of absorption and desorption at the different temperature are measured and a van's Hoff diagram is plotted, which are compared to those for pure LiBH4. In addition, the kinetics of absorption and desorption of destabilized LiBH4 will be discussed.

Modelling the Influence of the Temperature on the Subsurface Deformation of an Aluminum Pin during a Wear Test: Mario Rosenberger[1]; Elena Forlerer[2]; *Carlos Schvezov*[1]; [1]UNaM; [2]UA Materiales - GIDAT-GAEN. CNEA.

During the wear of aluminum pins under dry sliding it is normally observed a lot of plastically deformed material placed on the ending borders. This deformation is located mainly in the subsurface. The influence of the temperature on the subsurface deformation was studied using finite element analysis. A three-dimensional model was employed, and temperature dependent properties were assumed. Loads were applied simulating a test performed in a pin-on-ring machine. An elasto-plastic model was employed with small deformation in the plastic range. 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 comparison of these results with experiments performed on A1060 alloys reinforced with 15% alumina particles shows little deviation between predictions and experiments which may be attributed to the difference of mechanical properties between the alloys.

Modification of Cast IN738LC Alloy Microstructure: *Nader El-Bagoury*[1]; Mohamed Waly[1]; Adel Nofal[1]; [1]CMRDI

The microstructure of cast polycrystalline Inconel 738LC (IN738LC) under different heat treatment conditions was investigated. The cast microstructure of this alloy consists of austenitic γ matrix, γ' precipitates, MC carbide and γ/ γ' eutectic. The microstructure of the conventional solution treatment, 1120°C/2h/ accelerated air cooling (AAC), contains a bimodal γ' precipitate. Solution treatment at several temperatures of: 1120, 1180, and 1220?C for 1.5 h as well as 1180°C/1.5h + 1220°C/2h has been carried out under argon atmosphere. Accelerated air cooling (AAC) and water quenching (WQ) were applied after solution treatment. Moreover, aging treatment at 845°C was carried out for all solutioning conditions followed by WQ. Solution treatment at 1180°C/1.5h + 1220°C/2h gives the best homogeneity for different alloying elements and a uniform size for the fine γ' precipitates. AAC increases the volume fraction and tends to agglomerate γ' precipitates compared to WQ.

Nanotechnology Education: Pennsylvania's National Model: *Robert Ehrmann*[1]; [1]Pennsylvania State Center for Nanotechnology Education and Utilization

Pennsylvania has been working on meeting the critical need for nano-scale trained workers for the last ten years. The NSF Advanced Technology Education (ATE) Center at Penn State University and its partner institutions prepare students to work in any industry that uses micro- and nanotechnology. The Center's curriculum and facilities enable partner colleges across Pennsylvania to offer more than 35 associate degree programs in nanotechnology. The key feature of these degree programs in nanotechnology is the PA Nanofabrication Manufacturing Technology (NMT) Capstone Semester consisting of six hands-on courses taught three times per year. The Center's faculty, staff, and facilities provide an immersive experience in nanotechnology fabrication and characterization, for the community college and university students who come to Penn State University from their home colleges for the Capstone Semester. Capstone semester graduates are employed in micro- and nanotechnology jobs at nearly 100 companies from a wide variety of industries.

Novel Method for Identifying Low-Angle Sub-Grain Boundaries: *Kevin King*[1]; Benyue Liu[1]; Md. Zakaria Quadir[2]; Michael Ferry[2]; Lori Bassman[1]; [1]Harvey Mudd; [2]University of New South Wales

Post-processing of EBSD slice data for 3D reconstruction of crystallographic volumes requires boundary identification for regions of interest. In the case of subgrain structures such as microbands, these boundaries are low-angle, and automatic, accurate identification of regions presents a number of challenges. In commercial software, misorientations between individual pixels are used to identify boundaries; however, with subgrains there are instances of gradual orientation change. By using a novel method that combines a color quantization algorithm and misorientation between pixels, we can more accurately identify regions. Minimum variance color quantization identifies a specified number of major components within an inverse pole figure to create a quantized map. This method provides an alternative way to group similar orientations. As an example, we applied this method to microbands in deformed IF steel. The 3D reconstruction allows us to gather statistical data for local normals corresponding to slip systems active in the deformationprocess.

Novel Method for Physical Simulation of Solidification Process in Slab Continuous Casting: Jianping Liang[1]; Yulai Gao[1]; Renxing Li[1]; *Qijie Zhai*[1]; [1]Shanghai University

Physical and numerical simulations of continuous casting processes are general approaches to avoid costly and heavy experiments on full-scale production lines. In the present work, a novel approach based on improved Bridgeman method is presented to physically simulate the solidification process of slab continuous casting. Attributing to the similarity of the heat transfer between unidirectional

solidification and practical slab continuous casting process, the Bridgeman setup was improved with real time controlling of draw speed, heating temperature and cooling rate, then growth velocity of crystals and overheat of melt were online controllable. During the simulation, the solidification parameters were set according to that of the practical slab continuous casting, by which the so called physical simulation was performed. Utilizing this novel method, the slab solidification process of AISI 321 stainless steel was simulated, showing good agreement with the practical production in solidification structure.

Numerical Simulation of Phase Decomposition during Aging in Cu-Ni Based Alloys: Erika Avila-Davila[1]; *Victor Lopez-Hirata*[1]; Dulce Melo-Maximo[1]; Maribel Saucedo-Muñoz[1]; Orlando Soriano-Vargas[1]; Jorge Gonzalez-Velazquez[1]; [1]Instituto Politecnico Nacional

The microstructure simulation of spinodal decomposition was carried out in the isothermally-aged Cu-Ni and Cu-Ni-Fe alloys using the phase field method. The calculated results were compared to those determined by atom-probe field ion microscope analyses of the solution treated and aged alloys. The numerically simulated results of the concentration profiles and microstructure showed a good agreement with the experimental ones in both alloy systems. A slow growth kinetics of phase decomposition was observed to occur in the early stages of aging in both alloys. The morphology of decomposed phases consisted of an irregular shape with no preferential alignment in any crystallographic direction at the early stages of aging in the aged alloys. In the case of the aged Cu-Ni-Fe alloys, a further aging caused the change of initial morphology to an equiaxial shape of the decomposed Ni-rich phase aligned in the elastically-softest crystallographic direction <100> of Cu-rich matrix.

Numerical Simulations of the Crimping Process: *Tobias Rist*[1]; [1]Fraunhofer Institute for Mechanics of Materials IWM

Crimping is an important process to manufacture electrical connectors by deforming one or more metals to hold together. The increasing number of electrical components in automobiles makes crimp connections very important parts, the reliability of which must be assured. Simulation of process and operation is an efficient tool to optimize crimped connectors and to reduce the amount of expensive testing during development of new crimps. A three dimensional FE-Model validated with crimp experiments is used to simulate the crimp process. Therefore tensile tests on clip and wire material were performed to determine the parameters of the material models employed in the process simulations. The Calculations lead to various process dependent results like crimp force, contact pressure and resulting stress state that give information about the crimp performance. Thus, a significant reduction in cost and development time can be achieved.

Nylon 6/Brazilian Clay Nanocomposites: Evaluation of Thermal Behavior by Differential Scanning Calorimetry and Heat Distortion Temperature: Rene Paz[1]; Amanda Melissa Leite[1]; *Edcleide Araujo*[1]; Tomas Melo[1]; [1]Universidade Federal de Campina Grande

Recently, investigation of nanocomposites made from polymers and silicate/ layers has received significant attention because often they exhibit improved mechanical properties, thermal, optical and physical when compared with conventional or polymer composites. In this work, nanocomposites were prepared using Brazilian clay and a quaternary ammonium salt. The used nylon6 matrix was with three different molecular weight and the thermal properties were evaluated. The results of DSC showed discrete changes in temperature and enthalpy than that nylon 6. In general, the nanocomposites exhibited bigger degree of crystallinity compared to pure nylon 6. The heat distortion temperature (HDT) of the nanocomposites was around 550°C and the nylon6 around 490°C. This increase was attributed to good dispersion of the layers of silicate in the nylon6 matrix.

Nylon6/Ferrite Composites for Absorbers of Electromagnetic Radiation: Daniella Bezerra[1]; Keila Machado de Medeiros[1]; Taciana Regina de Gouveia[1]; *Edcleide Maria Araújo*[1]; Ana Cristina Figueiredo de Melo Costa[1]; [1]UFCG

Composite consists of a mixture or combination of the two or more, micro or macro constituents that differ in shape and chemical composition and, in essence, are insoluble in one another. The nylon is a polymer that presents dimensional stability, good resistance to impact without notch and excellent chemical resistance. Already the ferrites are absorbers of electromagnetic radiation and have versatility to be used as a composite of ferrites. The nylon6/ferrite composite was obtained by mixing 10, 20, 30% of ferrite added to nylon6 in a blender internal Haake. The objective of this work was to develop nylon6/ferrite composite to achieve superior properties or better in some aspects regarding the properties of each of its components. The results were very promising, with a good interaction between the ferrite and nylon6, to be used as absorbers of electromagnetic radiation.

Observation of Solid-State Wetting Morphology in Abnormally Growing Grain of Fe-3%Si Steel: *Kyung Jun Ko*[1]; Jong Tae Park[2]; Jae Kwan Kim[2]; Anthony D. Rollett[3]; Nong Moon Hwang[1]; [1]Seoul National University; [2]POSCO; [3]Carnegie Mellon University

In this study, we suggest a new approach to the growth advantage of abnormal grain growth (AGG) by solid-state wetting. If the energy sum of the two grain boundaries is lower than the energy of the other grain boundary in contact at the triple junction, the high energy grain boundary will be replaced by the two low energy grain boundaries through the wetting process. The experimentally-observed abnormally growing grain by solid-state wetting has the microstructural feature of AGG such as the formation of numerous island and peninsular grains. Very high frequency of island and peninsular grains formed at or near the growth front of abnormally growing grains could be best explained by solid-state wetting. 3-sided or 4-sided grains with negative curvatures, which are formed near the growth front of abnormally growing grains, are the two-dimensional section vertical to the triple junction wetting in three-dimensional polycrystalline structure.

Optimization of Machine Parameters for an A487 Steel Welding Process: *Armando García*[1]; Mario Trejo[1]; Mauricio Garza[1]; Jorge Acevedo[1]; [1]Corporación Mexicana de Investigación en Materiales S.A. de C.V., Ciencia y Tecnología

Aim of this work is to show relation between machine parameters in a GMAW process and weld depth on an A-487 steel. Industrial application of this steel is well known for heavy work. Artificial intelligence and statistical approaches are carried to find optimal parameters for deep weld penetration.

Optimization of Milling Conditions for the Production of Fine Silver Powders: *H. Kübra Yumakgil*[1]; Hasan Gökçe[1]; Burak Özkal[1]; Sebahattin Gürmen[1]; M. Lütfi Öveçoglu[1]; [1]ITU

High energy milling of ductile metals is difficult because of their flattening tendency under milling deformation. These powders are easily cold welded to each other and get flattened. Therefore to ensure their continues fragmentation is a complex process which needs optimization of milling parameters and in most cases it is necessary to add process control agents. Silver is a good example having above mentioned difficulties. In this study high energy milling behavior of Ag powders were studied under different milling conditions. Milled powders were characterized via XRD, BET, LPS measurements and SEM observations for the optimization of the milling conditions for achieving continues fragmentation Ag powders leading fine powders.

Oxidation Behavior of Low Carbon Steel in Oxygen and/or Water Vapor at 500-700°C: *Jei-Pil Wang*[1]; W.D. Cho[1]; [1]University of Utah

The oxidation behavior of low carbon steel was investigated at 500-700°C in the oxidizing atmosphere with or without water vapor. The effects of temperature, oxygen pressure, and water vapor contents on the oxidation of the steel were studied. The morphology and microstructure of oxide formed in dry or moist oxygen was examined and analyzed by XRD, SEM, and EDX. The oxidation mechanism was discussed based on the study of diffusion, oxide defects, and microstructure between the substrate and oxide layer.

Partial Oxidation on Methane on Ni/Ceria-Based Materials: *Maria Salazar-Villalpando*[1]; [1]National Energy Technology Laboratory

Partial oxidation of methane (POM) was studied over Ni/(Ce0.56Zr0.44)O2-x, Ni/(Ce0.91Gd0.09)O2-x, Ni/(Ce0.71Gd0.29)O2-x and Ni/(Ce0.88La0.12)O2-x. The effect of catalyst reducibility and redox cycles was investigated. It was found that the type of doped-ceria support and its reducibility played an important role in the catalyst activity. It was also observed that redox cycles had a positive influence on H2 production, which was enhanced as the number of redox cycle increased. Results of carbon formation are discussed as a function of ionic conductivity. Temperature programmed reduction (TPR) profiles, and XRD patterns were determined to characterize catalysts. Experimental tests to determine the catalytic activity revealed that of the materials tested, Ni/(Ce0.56Zr0.44)O2-x wasthe most active material for the production of syngas, which correlates with its TPR profile. It was observed that doping CeO2 with Zr, rather than with La or Gd caused an enhanced reducibility of Ni/supported-ceria catalysts.

Photocatalytic Reduction of CO2: A Review: *Maria Salazar-Villalpando*[1]; Bryan Reyes[1]; [1]National Energy Technology Laboratory

The transformation of CO2 to hydrocarbons using sunlight is one of best routes to produce renewable energy. State of the art of the photo catalytic reduction of CO2 with H2O will be discussed here. Several types of catalysts have been used to study this reaction, for example: Ruthenium dye-sensitized TiO2-based catalysts; TiO2/SO42– photo catalyst; copper-doped Titania catalysts, etc. The discussion of results will include identifying the effect of type catalyst and type of reactor on composition of products and yield of reaction. Main reaction pathways will be reviewed; thermodynamic and kinetics effects will be discussed. Recommendations to improve the yield of reaction will be included.

Pilot Experiments of Low Temperature (700 ~ 800°C) Aluminum Electrolysis in a 5kA Aluminum Reduction Cell: *Huimin Lu*[1]; Hengchao Zhao[1]; Pengkai Wang[1]; [1]Beijing University of Aeronautics & Astronautics

In this paper, pilot experiments of the new technique of low temperature (700 ~ 800°C) electrolysis in a 5kA aluminum reduction cell are conducted. The electrolyte is the Na3AlF6-AlF3-BaF2-CaF2 bath system. The experiment results indicate that the Na3AlF6-AlF3-BaF2-CaF2 bath system is promising. These pilot experiments lay a good foundation for industrial application. In the meantime, the physico-chemical properties of Na3AlF6-AlF3-BaF2-CaF2 bath system were systematically studied based on experiments designed using three-factor quadratic orthogonal regressive method. The cathodic current efficiency of the new low temperature aluminum electrolysis is up to 94% and DC power consumption 12000kWh/t aluminum in 5kA experiments cell.

Polymer-Based TNT Sensor Using Initiated Chemical Vapor Deposition: *Lucas McIntosh*[1]; [1]Missouri University of Science and Technology

Current techniques for the detection of nitroaromatic high explosives such as 2,4,6-trinitrotoluene (TNT) are considered inadequate for their expense and/or inconvenience in field operations. Our goal is to develop a mechanically robust, low power, highly sensitive and selective polymer-based TNT sensor that can be incorporated into a field-ready detection system. Such a system would rely on the polymer swelling as a result of absorption or reaction with TNT, thus closing a DC electrical circuit. Various homo- and co-polymers hypothesized to interact with the aromatic ring and nitro groups of TNT were deposited on silicon wafers using a novel polymerization technique – initiated chemical vapor deposition (iCVD). Using in situ interferometry to monitor swelling, samples were found to swell by as much as 800% in the presence of TNT analogues such as 4-nitrotoluene at a concentration of 187 ppm. Samples did not interact with controls such as water, nitrogen, and cyclohexane.

Post-Consumption Decoloration Oil Application as Biofuel Using Brazilian Clay: Elaine Araújo[1]; *Edcleide Araújo*[1]; Marcus Fook[1]; Renata Barbosa[1]; Sara Oliveira[1]; [1]UFCG

Since the ancient times, clays were used as decolorant material for various types of oils. These clays were called “decolorant clay”. They have the property to decolor dye materials present in mineral oils, plants and animals. Biofuel is a fuel derived from biomass of live organisms. As biodiesel is produced from renewable sources, the generation of employment due to industrial scale production may cause a reduction in the dependence on foreign diesel importing, as well as the reduction of air pollution by the addition of biodiesel to diesel. This study aimed to develop a technological process to decolor post- consumption oil to be applied as biofuel. The clays and oils were characterized by XRD (X-ray Diffraction), FTIR (Fourier Transform Infrared) and X-ray fluorescence. It was observed that the post-consumption oils presented a higher decoloration result after treatment with the Brazilian clay.

Precipitation during Ausaging and Composition Design for Ferromagnetic Shape Memory Effect of Fe-Ni-Co-Ti Alloys: Jin Mingjiang[1]; *Jin Xuejun*[1]; [1]ShangHai Jiao Tong University

Fe-Ni-Co-Ti alloys have received attention for its potential magnetically induced shape memory effect (MISME) with high output power and excellent mechanical properties. Present study is concerning on optimizing composition and ausaging technique to obtain the thin-plate-martensite at room temperature,which is critical for promising MISME, through the adjustment of transformation temperature and matrix strength. Morphology of martensite in different composition and ageing process were presented and the influence of component in alloy was investigated. Hardness and MS temperature are also tested as a function of ageing time. Results show that nickel is the sensitive element on morphologies of martensite and MS temperature. With Ni content of 29~32wt% and appropriate aging treatment, the thin plate martensite could be obtained at room temperature. Ti plays an important role in improving hardness in the process of precipitation, while Co accelerates the Ni3Ti precipitate. The impact of precipitation on martensitic transformation is also discussed.

Precipitation Kinetic of AlMgSi Alloy Added with Ag: *S. Valdez*[1]; Said R. Casolco[1]; [1]ICF-UNAM

AlMgSi alloy is widely attractive due to their physical, mechanical and chemical properties, such as corrosion, formability, weldability, etc. However, a study detailed on the kinetic precipitation with Ag addition has not been carried out yet. In addition, the Ag content could be exerting a marked effect on their mechanical properties and dimensional stability. The present work reports the silver effect on the hardenable AlMgSi (6xxx) alloy. In addition, the age hardening capability and their relationship with the Ag-alloying addition influence, has been studied. The results describe the kinetic of precipitate formation and cluster dissolution during the ageing. The phase transformation was observed by diferential scanning calorimetry (DSC) and X-ray diffraction XRD. The formation of atomic clusters was identified before the GP-zone and precipitate formation. A β-phase precipitates were formed during the age at 190°C. The silver added improves the precipitation kinetic and microhardness value.

Precipitation Kinetics in Cerium Nitrate Precursor Ddroplets Heated by Mmonochromatic Irradiation: *Saptarshi Basu*[1]; Abhishek Saha[1]; Sudipta Seal[1]; Virendra Singh[1]; [1]University of Central Florida

Generation of nanoceria coating from liquid cerium nitrate precursors involves injection of precursor containing droplets into a high temperature plasma environment. Upon vaporization, nucleation, precipitation and shell fracture the final microstructure of the coating is attained. To investigate the precipitation mechanism for cerium nitrate precursors, they were heated by a CO2 laser to simulate the rapid heating condition the droplets encounter in a plasma. Ex-situ analysis of the laser-heated samples were carried out using SEM and XPS.In situ analysis involved high speed imaging to study the morphological changes in the droplet before and after precipitation. It is seen that depending on the solute loading concentration, laser heating of the droplets can give rise to very dense to porous type of precipitates. The high speed imaging show the evolution of the droplet morphology which included contraction in size, instability in the liquid phase, vapor bubble formation, nucleation and precipitation.

Precision Forging of a Two Cylinder Crankshaft: *Sven Muller*[1]; [1]Institut für Integrierte Produktion

Precision forging is defined as a flashless near net shape forging. A quality in the tolerance class from IT 8 to IT 10 can be achieved. The flashless precision forging offers an integrated heat treatment with the forging heat, because a clipping process is not necessary. After the forging and heat treatment often only a final fine machining of the functional surface with small chip volume is required. In the collaborative research project SFB 489 a two-cylinder-crankshaft is selected as an example for complex flat long pieces with a characteristic mass distribution along the longitudinal axis. The continuative development considers the thermal and mechanical tool stresses, which are also as complex as the crankshaft itself. Further on a parameter study on a bi-directional forging tool is made. The tests of the forging sequence, tools, cooling systems and measuring technology of the developed process are finished now.

Prediction of Microstructural Changes in Drawing of Pearlitic Steel Wires: *Yong-Shin Lee*[1]; W-J Nam[1]; Kyung-Tae Park[2]; [1]Kookmin University; [2]Hanbat University

It is well known that fully pearlitic steel wire manufactured by cold drawing exhibits very high strength. However, its ductility is often limited by the internal defects during drawing. It is generally accepted that interlamellar spacing is the most important factor to control ductility and strength of pearlitic steels, simultaneously. It is attempted to predict the microctructural changes during drawing of a pearlitic steel wire. First, finite element simulations for wire drawing are performed to trace the deformation histories of material points in a steel wire. Then, a couple of algorithms developed in this work are applied to predict changes of microstructures such as orientation, shape, and thickness of a cementite. The predictions will be compared to those reported in the literature. Also, the difference of microstructural evolution according to the depth from the surface in the cross-section of the wire will be carefully investigated.

Preparation and Characterization of Assymetric Membranes Obtained of Nylon6/Brazilian Clay Nanocomposites: Amanda Melissa Leite[1]; Larissa Maia[1]; *Edcleide Araújo*[1]; Hélio Lira[1]; [1]Universidade Federal de Campina Grande

A membrane is an intherphase between two adjacent phases acting as a selective barrier, regulating the transport of substances between the two compartments. The main advantages of membranes technology as compared with other unit operations in chemical engineering are related to this unique separation principle, i.e. the transport selectivity of the membrane. Separations with membranes do not require additives, and they can be performed isothermally at low temperatures and compared to other thermal separation processes-at low energy consumption. In this work, asymmetric membrane of Nylon6/Brazilian clay nanocomposites using quaternary ammonium salts were obtained by phase inversion method. The membranes were characterized by SEM. The results showed that there is a significant difference in size and distribution of pores between pure nylon 6 membranes and membranes obtained from nanocomposites.

Preparation and Characterization of NiCo2O4 Fibre by Coordination Coprecipitation-Thermal Decomposition Method: *Zhan Jing*[1]; Zhang Chuanfu[1]; Bai Meng[1]; Wu Jianhui[1]; [1]Central South University

The spinel NiCo2O4 fibers with diameters less than 1um were prepared by thermal decomposition of nickel –cobalt oxalate complex precursor containing ammonium, which were obtained by coordination coprecipitation techinique. The effects of different Ni/Co ratios, decomposition temperature and decomposition time on the phase constitute of final product were addressed in detail. The crystallinity, purity, and surface morphology of the as-prepared NiCo2O4 fibers were investigated by XRD, IR, SEM, respectively. Finally, Structure of nickel cobaltite spinel examined by X-ray absorption spectroscopy (XPS) indicates, as expected, that Ni occupies the octahedral sites of the spinel structure while Co occupies both tetrahedral and octahedral sites. The result of the surface examination by xps shows that the surface composition is different from nominal bulk composition.

Preparation of Fibrous Nickel Powder by Complexing Precipitation-Thermal Decomposition Method: *Jianhui Wu*[1]; Chuanfu Zhang[1]; Jing Zhan; Youqi Fan[1]; Baiyun Huang[1]; Yuehui He[1]; [1]Central South University

Fibrous nickel powder was prepared by complexing precipitation - thermal decomposition method. The composition and morphology of the powder were characterized by the analysis methods of XRD and SEM. The effects of temperature, concentration, pH value and surfactant on the morphology and the dispersion of the precursor and the conditions of the thermal decomposition on the morphology and the dispersion of the nickel powder have been studied. The results indicate that the nickel powder is fibrous and well dispersive, and can be prepared by thermal decomposition of the precursor, which is obtained under conditions as proposed: precipitation temperature is 60~70°, the nickel ion concentration is 0.5~0.8 mol•L^{-1}, pH value is 8.4~8.8 and adding PVP as surfactant.

Preparation of Zinc Oxide Nanostructures from Zinc Sulfate and Zinc Nitrate Precursor: *Sebahattin Gurmen*[1]; Burcak Ebin[1]; Burak Ozkal[1]; [1]Istanbul Technical University

Over the past decades, zinc oxide nanostructures have attracted great interest due to its unique physical and chemical properties including optical transparency, electric conductivity, and light emission. However, size and morphology are important parameters to determine the physicochemical features of ZnO nanostructures. Ultrasonic spray pyrolysis method, suitable for formation of spherical particle morphology, was used to prepare nanostructure ZnO particles from zinc sulfate and zinc nitrate solution. The size and shape of the ZnO particles were controlled by the reaction conditions, temperature, selection of precursors, frequency of ultrasonic atomizer, carrier gas kind and flow rate. Effects of temperature and precursor concentration on products were investigated in this study under constant gas flow rate and frequency. Characterization studies were conducted on not only size and shape morphologies, but also crystalline structure, and phase determination. Obtained particles size increases with elevated reaction temperature, and particle morphology strongly depends feature of precursor.

Preparation of ZrB2-ZrC Composites by Spark Plasma Sintering: *Filiz Sahin*[1]; Ipek Akin[1]; Onuralp Yucel[1]; Takashi Goto[2]; Gultekin Goller[1]; [1]Istanbul Technical University; [2]Tohoku University Institute for Materials Research

The ZrB2-ZrC composites were prepared by the spark plasma sintering (SPS) at temperatures of 1800 to 2000°C for 300 under a pressure of 50 MPa. Densification, crystalline phases, microstructure and mechanical properties of the ZrB2-ZrC composites were investigated. Fully dense ZrB2-ZrC composites containing 20 to 80 wt% ZrC with a relative density of more than 98% were obtained at 1900°C for 300 s. The all characteristics peaks of ZrB2 and ZrC were identified and chemical reaction was not detected between ZrB2 and ZrC for all compositions at 1800 to 2000°C. Vickers hardness of dense ZrB2-SiC composites containing 80 wt% ZrC sintered at 1900 and 2000°C had the maximum value of 18.7 GPa. The highest fracture toughness of 3.5 MPa•m1/2 was observed for ZrB2-ZrC composite containing 80 wt% ZrC sintered at 1900°C.

Processing of a TiAl Alloy by Powder Metallurgy and Hot Working: *Rao Kamineni*[1]; Y.V.R.K. Prasad[1]; [1]City University of Hong Kong

Titanium aluminides have superior high temperature properties and are attractive for gas turbine applications. Cast titanium aluminides have large grain sizes which reduce hot workability. Alternately, powder metallurgy technique is explored by mixing of elemental powders for 2 hrs to prepare 46Ti-46Al-4Nb-2Cr-2Mn followed by Hot Isostatic Pressing (HIP) at 1150°C for 4 hrs under a pressure of 150 MPa. In addition to the formation of TiAl solid solution, the microstructure showed a small volume fraction of Nb-rich phase. The HIP'ed billets were compressed at temperatures and strain rates in the ranges of 850-1050°C and 0.0001-10 s^{-1}. The flow curves exhibited continuous flow softening at strain rates lower than 0.1 s^{-1} while fracture has occurred at higher strain rates. The hot workability was good at temperatures higher than 1000°C and the flow stress at different temperatures and strain rates follows the kinetic rate equation.

Production and Characterization of Soda-Lime Photosensitive Glasses: *Arca Iyiel*[1]; Suheyla Aydin[2]; Onuralp Yucel[2]; [1]Turkiye Sise ve Cam Fabrikalari A.S.; [2]Istanbul Technical University

Photosensitive glasses can be produced by conventional methods but contain alkali halide silver (AgX), alkali oxide, fluorine and at least one of the group consisting of chlorine, bromine and iodine, after an exposure to high energy or actinic radiations following a unique heat treatment. In this study, previously known sodium silicate photosensitive glass composition was modified to conventional soda-lime float glass composition which contains silver, alkali oxide, fluorine and halide group elements. Then by means of the applied UV radiation microstructural and optical properties have been controlled with the aid of the additives. The effect of lantanides at colorless level, on the photosensitive glasses are studied. The present study shows the effects of addition of lantanides such as Ho2O3, Er2O3, Pr2O3, Nd2O3 for first time. Optical characterization has been also performed before and after UV exposure. Microstructural changes after the photochemical process were observed clearly.

Production and Characterization of ZrB2-ZrC-SiC Composites: *Gultekin Goller*[1]; Ipek Akin[1]; Filiz Sahin[1]; Onuralp Yucel[1]; Takashi Goto[2]; [1]Istanbul Technical University; [2]Tohoku University

In this study, the production of ZrB2-ZrC-SiC composites using spark plasma sintering (SPS) technique was studied. Sintering of powder mixtures was carried out at 1850 and 1900°C for 180 to 300 s under a uniaxial pressure of 50 MPa in vacuum atmosphere. The temperature of the die was increased at 1.7°C/s. Shrinkage of the specimens during SPS process was continuously monitored. Densities of the composites were determined by the Archimedes' method and more than 98% relative density was obtained for the composites. The crystalline phases of the specimens were identified by X-ray diffractometry. Vickers hardness (HV) was measured under loads of 0.98 to 9.80 N and fracture toughness (KIC) were evaluated by a microhardness tester. The fracture toughness was calculated from a half length of crack formed around the indentations.

Properties and Consolidation of Nanostructured MoSi2 from Mechanically Reacted Powder by Rapid Sintering: In-Jin Shon[1]; *Jeong-Hwan Park*[1]; Kee-Do Woo[1]; Jin-Kook Yoon[2]; [1]Division of Advanced Materials Engineering, the Research Center of Industrial Technology, Chonbuk National University; [2]Advanced Functional Materials Research Center, Korea Institute of Science and Technology

MoSi2 has been investigated as potential material for high temperature structural applications and for application in the electronics industry. Its properties provide a desirable combination of a high melting temperature (2020°C), high modulus (440 GPa), good oxidation resistance in air, a relatively low density (6.24 g/cm3). A dense nanostructured MoSi2 was sintered by the high-frequency induction heating method within 1 minute from high energy ball milled powder of MoSi2. Highly dense MoSi2 with relative density of up to 97% was produced under simultaneous application of a 60 MPa pressure and the induced current. The average grain size of MoSi2 was about 100 nm. The hardness and fracture toughness values obtained were 1203 kg/mm2 and 4.2 MPa•m1/2, respectively. These fracture toughness and hardness values of nanostuctured MoSi2 are higher than those (fracture toughness; 2.58 MPa.m1/2 hardness; 8.7Mpa) of micronstuctured MoSi2.

Rapid Synthesis and Consolidation of Nanocrystalline 1.5Ti-Al2O3 from Mechanically Activated Powders: Dae Ho Rho[1]; In-Jin Shon[2]; *Byung-Ryang Kim*[3]; Kee-Do Woo[3]; Jin-Kook Yoon[4]; [1]Department of Metal Processing Research Center, Korea Institute of Science and Technology; [2]Division of Advanced Materials Engineering, the Research Center of Industrial Technology, Chonbuk National University; [3]Division of Advanced Materials Engineering and Research Center for Advanced Materials Development, Engineering College, Chonbuk National University; [4]Advanced Functional Materials Research Center, Korea Institute of Science and Technology

Interest in cermet of Ti-Al2O3 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 hardness. Dense nanocrystalline 1.5Ti-Al2O3 composite was synthesized by pulsed current activated combustion synthesis(PCACS) method within 2 min in one step from mechanically activated powders of 1.5TiO2 and 2Al. Highly dense 1.5Ti-Al2O3 with relative density of up to 99% was simultaneously synthesized and consolidated under application of a 60 MPa pressure and the pulsed current. The average grain sizes of Ti and Al2O3 in the composite were 282nm and 65 nm, respectively. The hardness and fracture toughness of the composite were 1207 kg/mm2 and 7 MPa.m1/2, respectively.

Rapid Transient-Liquid-Phase Bonding of Al_2O_3 Ceramics: *Thomas Reynolds*[1]; Sung Hong[1]; Christopher Bartlow[1]; Andreas Glaeser[1]; [1]University of California-Berkeley

In engineered devices, dissimilar materials must often be joined to attain desired properties. Transient-liquid-phase (TLP) bonding is an elegant method of joining materials at reduced temperatures to protect fragile microstructures, but it often requires multi-hour isothermal holds. In the present work, the processing time to join high-purity Al_2O_3 is significantly reduced using Ni/Nb/Ni multilayer interlayers that form thin transient-liquid films. We demonstrate that ultrahigh strengths, averaging $\geq$ 500 MPa, are attainable with isothermal holds as short as 5 min at 1400°C. The wetting behavior of the TLP on Al_2O_3, the rapid redistribution of Ni within the interlayer, and the joint fracture characteristics are described. Using multilayer interlayers with similar thermokinetic properties, it should be possible to extend this joining technology to other materials.

Relaxed Grain Cluster Homogenization Scheme for Polycrystals: *Denny Tjahjanto*[1]; Philip Eisenlohr[1]; [1]Max-Planck Institut für Eisenforschung

We develop an efficient and accurate homogenization scheme, namely relaxed grain cluster (RGC). The scheme is based on the generalization of the relaxed constraints Taylor model. A cluster consisting of eight uniform hexahedral grains is considered. The relaxation of local deformation of individual grains is described by means of interface relaxation vectors. The kinematic of the relaxation is formulated within a finite deformation framework. An penalty associated with deformation incompatibility at interfaces is computed in analogy to the concept of geometrically-necessary dislocations. The relaxation vectors are determined in accordance with the minimization of the total energy, which leads to the condition of the stress equilibrium at the interfaces. Several elementary simulations have been performed. The predictions of the relaxed grain cluster model in terms of the effective stress-strain response is analyzed. In addition, the RGC scheme is used to simulate texture evolution during rolling.

Removal of Impurity Elements from the Molten Aluminum: Modeling and Validation: *Xuewei Lv*[1]; Lifeng Zhang[1]; Chenguang Bai[2]; [1]Missouri University of Science and Technology; [2]Chongqing University

In order to remove the impurity elements from the molten aluminium, many processes, such as using the inert gas, reactive gas, reactive powders, unreactive powders, slag, vapor pressure, or their combinations, have been used during recent thirty yeas. In the current paper, mathematical models for these refining methods were developed. The removal of impurity elements for batch and continuous reactor were investigated. The modeling was validated by the industrial measurement. The effect of the parameters, such as the refining temperature, gas flow rate, powder injection rate, stirring power, removal efficiency of the impurity elements were discussed.

Removal of Pb, Cd and Cl from Waelz Oxide via Pyrometallurgical Process: *Hakan Morcali*[1]; Bora Derin[2]; Adnan Aydin[1]; Onuralp Yucel[2]; [1]Marmara University; [2]Istanbul Technical University

In this study, removal of residue such as, chlorine, lead and cadmium was carried out via pyrometallurgical process by using collected condensed powder (Waelz oxide). In the previous study, Waelz oxide (containing 66.24 wt. % Zn, 0.18 wt. % Fe, 5.55 wt. % Pb, 0.0859 wt. % Cd, and 4.99 wt. % Cl) was collected through carbothermic reduction of EAF dust at 1100°C for 90 minutes. In the experimental series, a temperature controlled pilot scale rotary furnace was utilized. Temperature (1000, 1100, 1150, and 1200°C) and time (0-120 minutes) were selected as reaction parameters. It was observed that the amount of lead, cadmium and chlorine in the Waelz oxide decreased with increased both time and temperature. The optimum conditions for the removal of Pb, Cd and Cl were achieved at 1200°C for 120 minutes. As a conclusion, zinc oxide with 99.04% purity was obtained after the refinement by volatilization process. The products obtained were characterized by X-Ray diffraction and chemical analysis techniques.

Removal of Sr (II) from Aqueous Solutions by Using Bentonite as Natural Adsorbent: *Siavash Nikfar*[1]; Saeed Milani[2]; Sharyar Mirhakimi[1]; [1]Arak Azad University; [2]Nuclear Science Research School, Nuclear Science and Technology Research Institute

In the present study, the ability of bentonite (clay ,as natural adsorbent) to remove strontium ions from aqueous solutions has been investigated. Batch method was carried out during adsorption process. The effect of various parameters such as contact time, initial concentration, PH, particle size and existence of competing metal ions has been studied. Kinetic of adsorption showed that the uptake of strontium ions is very rapid during first thirty minutes and equilibrium time is independent of initial strontium concentration. Simple kinetic and thermodynamic models have been applied to the rate and isotherm sorption data and the relevant kinetic and thermodynamic parameters were determined from the graphical presentation of these models.

Semiconducting Properties of Passive Films and Pitting Corrosion Resistance of Nickel Free High Nitrogen Austenitic Stainless Steels: *Huabing Li*[1]; Zhouhua Jiang[1]; Yan Yang[1]; Yang Cao[1]; [1]Northeastern University

The semiconducting property of passive films of nickel free high nitrogen austenitic stainless steel was investigated in chloride solution by electrochemical impedance spectroscopy. The structure, chemical composition of passive films and the pitting corrosion of the steels have been investigated. The capacitance results show that the passive films behave as n-type and p-type semiconductors in the potential range above and below the flat band. The donor density, acceptor density and the flat band decrease with increasing nitrogen. The thickness of the space charge layer of n-type semiconductor increases with increasing nitrogen. The steels exhibit excellent pitting corrosion resistance, and their pitting potentials and critical pitting temperature increase with increasing nitrogen in steels. The XPS results show that the beneficial effect of nitrogen on improving pitting corrosion resistance are attributed to the enrichment of nitrogen in passive films to form the ammonium ions and the synergy effect between molybdenum and nitrogen.

Semiconducting Properties of Passive Films of Nickel Free High Nitrogen Aaustenitic Stainless Steels: *Huabing Li*[1]; Jiang Zhouhua[1]; Yang Yan[1]; [1]Northeastern University

The semiconducting property of passive films of nickel free high nitrogen austenitic stainless steel was investigated in 3.5% wt NaCl solution by

electrochemical impedance spectroscopy (EIS). The capacitance results show that the passive films behave as n-type and p-type semiconductors in the potential range above and below the flat band (EFB). The donor density (ND), acceptor density (NA) and the EFB decrease with increasing the nitrogen content in steels. The thickness of the space charge layer(W) of n-type semiconductor increases with increasing the nitrogen content. The XPS results show that the passive films are composed of an inner region of a mixed chromium-iron oxide and an outer region of iron oxide. The nitrogen enriches on the out layer of passive films as the form of CrN, NH3, N(atom) and NH4+. The synergism effect between molybdenum and nitrogen improves greatly the pitting corrosion resistance of the high nitrogen stainless steels.

Sheared Slugs for Precision Forging – Improved Shear Zone Quality by an Oscillating Shear Cutter: *Michael Lücke*[1]; Karsten Müller[1]; [1]IPH - Institute for Integrated Production Hannover

Closed-die-forging requires constant process provisions. One of the most important factors of influence by forging without flash is the mass constancy of the billet. Because of large reachable quantities and low costs is the shearing of bar stock an established proceeding in the forging industry. Furthermore offers this method a nearly lossless process. Drawbacks of shearing are shearing faults and the inconstant volume of the sheared billets. For flashless forging in closed dies is the constancy of billet-geometry and -volume essential. Hence the IPH – Institute for Integrated Production worked in research projects on methods to enhance the cutting-plane-quality. A previous working of IPH shows that an oscillating cutter can improve the shearing output. In this study a provisional experimental set-up was used. To evidence these results, a new oscillating unit will be implanted into the shear. The existing solution interrupts the outgoing oil flow to 40 times per second.

SiC Particulate Reinforced Iron Matrix Composites Processed by Specimen Current Heating Hot Press Sintering: *Wang Yaomian*[1]; Zong B. Y.[1]; Yang Yufang[1]; Li Jie[1]; [1]Northeastern University

Specimen current heating hot press sintering is one kind of efficient technology to fabricate metal matrix composites. By use of Joule heat and hot pressing while intense current passing through the specimen, powder compact can be consolidated quickly. The whole sintering process is finished within a few minutes, thus the severe reaction between particle reinforcement and matrix is avoided. The results demonstrate that the two-stage sintering of this technology can improve material properties significantly comparing with the previous single stage sintering. The heating up time and holding time have important influence on the material properties during the two-stage sintering. The 10v% SiCp/Fe composites processed by the two-stage sintering with 100 seconds heating and 200 seconds holding can be achieved a density nearly to the theoretical value, the Brinell hardness to 477HB and the tensile strength being up to 915MPa.

Sintering Advances in Consolidating W and Its Alloys: *Avijit Mondal*[1]; Anish Upadhyaya[1]; Dinesh Agrawal[2]; [1]Indian Institute of Technology Kanpur; [2]The Pennsylvania State University

Microwave processing has been emerging as an innovative and highly effective sintering method offering many advantages over conventional methods for consolidation. It is recognized for its various advantages, such as: time and energy saving, very rapid heating rates, considerably reduced processing cycle time and temperature, fine microstructures and improved mechanical properties, better product performance, etc. Major constraints in conventional sintering of refractory material such as tungsten and its alloys , normally require high sintering temperatures, long soaking times favoring abnormal grain growth which finally leads to poor mechanical properties. This problem gets further aggravated at smaller (submicron and nano) tungsten powder sizes. This study describes recent research findings wherein pure tungsten and its alloys have been successfully consolidated using microwave heating which resulted in an overall reduction of sintering time of up to 80%. This sintering time compression restricts grain coarsening and results in superior mechanical properties.

Solute Concentration Effect on the Dendritic Orientation of Al-Sn Binary Alloy: *Jeong Yun Choi*[1]; Paul Matlage[1]; Ralph Napolitano[1]; [1]Iowa State University

On the pattern formation of the solidification, the solute concentration is recently regarded as a possible factor which can largely affect on the orientation of growing phases. This leads the control of the orientation of solidification morphologies is possible by adjusting the concentration in the melt phase, whereas the solid phase has been believed to grow along with the primary crystallographic orientations. In this work, to clarify the quantitative effect of solute content on the anisotropy of the intrinsic properties of the interface between the growing crystalline phase and the melt phase, the dendritic growth orientations of Al-Sn binary alloy with different concentrations are observed using experimental directional solidification, and computationally simulated using the phase-field model. By comparing the anisotropy of the equilibrated phases with that of growing phases with different growth velocities, the effect of concentration on the anisotropy of the kinetic factor of the interfacial properties is examined.

Structural Strength Evaluation of a Carbody by Structural Analysis and Load Test: *Sung Cheol Yoon*[1]; Jeongguk Kim[1]; Chang Sung Jeon[1]; Won Kyung Kim[1]; [1]Korea Railroad Research Institute

This paper describes a carbody structural analysis and the result of its loading test. The purpose of this study is to evaluate the safety and functionality of the body structure operating under maximum load. Aluminum alloy was used as the body structure's material. The carbody of rolling stock is a principal structure supporting major equipment of underframe, roof, interior and passenger. So, the strength evaluation of this structure is important and can be the core technique in rolling stock analysis. Both structural analysis and loading test were performed under the condition based on "Performance Test Standard for Electrical Multiple Unit" with the reference code JIS E 7105. The test results showed that the body structure is safe and stable under the condition of designed load.

Structure Changes during Tempering of Quenched Fe-C Steels as Assessed by Electrical Resistivity Studies: *Donald Lesuer*[1]; Oleg Sherby[2]; Chol Syn[1]; [1]Lawrence Livermore National Laboratory; [2]Stanford Univ

Electrical resistivity measurements are a powerful experimental tool for understanding the structure of Fe-C steels. It is shown that the electrical resistivity of fully annealed Fe-C steel is solely dependent on the amount of iron carbide independent of its distribution. During tempering of quenched Fe-C materials, however, significant changes are observed. Resistivity changes with carbon content show distinctly different behavior above and below 0.6 wt% C. These changes are attributed to the different martensitic products that form and their differences in tempering response. In the high carbon region, the data has been analyzed in terms of a time-temperature parameter t·exp(-Q/RT). The activation energy for tempering was found to be 150 kJ/mole which is related to Fe atom interaction with carbide particles. The results also show significant influence of substitutional solute atoms and retained austenite on the tempering response. Results provide insight into the mechanisms of tempering.

Structure Refinement of 12wt.%Cr Ferritic Stainless Steel by Pulse Current: *Changjiang Song*[1]; Jianping Liang[1]; Qijie Zhai[1]; [1]Shanghai University

Due to low Cr and Ni content, 12wt.%Cr ferritic stainless steel is a cheap stainless steel but still has good corrosion resistance. Therefore, it will have good potential applications in many filed, such as automotive industry and chemistry industry, because of low cost. To improve its mechanical properties, this paper investigated the effects of pulse current on solidification structure of a 12wt.%Cr ferritic steel. Experimental results show that during the solidification course of 12wt.%Cr ferritic stainless steel, employing of pulse current can significantly increase the area ratio of equiaxed crystal and decrease the grain size. Moreover, increasing the frequency and density of pulse current can improve refinement effect.

Study of Effect of Silicon Resin over Capacitance on $TaMnO_2$ Devices under Room and Humid Environments: *Miguel Esquivel-Aguirre*[1]; Héctor Barrientos[1]; Sandra Padrón[1]; Juan Torres[1]; Juan Pérez-Medina[1]; Pablo Ruiz[1]; [1]Kemet De Mexico

Silicon resins have a wide usage in electronics industry, especially on passive components prone to absorb moisture from the environment. TaMnO2 capacitors molded with epoxy compound are not hermetically sealed and can be affected by the conditions in the environment. Significant changes on capacitance (~ 5% of capacitance reduction) happen when the silicon resins are added to the cathode of the capacitors. The effects of the silicon layers on the cathode are discussed in this paper. The efficiency of the moisture protection was analyzed based on silicon resin nature at different concentrations and studied using fluorescent inks. The microstructure has been characterized with Scanning Electron Microscope. The effects on capacitance and other electrical properties were measured using Frequency Scan Techniques.The stability of the electrical properties was measured after Humidity 85% / 85 °C Test with and without voltage.

Study of Properties Enhancement of Magnesium Diboride (MgB2) by TaB2 Doping via High Energy Ball Milling: *Richard Perez*[1]; Yenny P Cardona Quintero[1]; Pedro Vargas[1]; Oswald Uwakweh[1]; Eric E Hellstrom[1]; David Larbalestier[2]; Durval Rodrigues Jr.[3]; [1]University of Puerto Rico; [2]Florida State University; [3]University of San Paulo, Brazil

The study of superconductivity properties enhancement on MgB2 due to TaB2 doping at 2 and 5 at.% levels were carried out. High energy ball milling was used for the purposes of fostering mechanical alloying, generation of nanometer sized particles, and strain inducements respectively. SPEX processed materials revealed smaller particle size and higher strains in comparison to the Pulverisette-4 processed ones. The 5 at.% TaB2 doped MgB2 yielded the highest critical current density (Jc) corresponding to 474.1 kA/cm2 at 2 T, while 344.4 kA/cm2 for SPEX and Pulverisette-4 materials. Correspondingly, the values of the flux pinning (Fp) deduced for the 5 at.% TaB2 doped MgB2 processed with the SPEX mill was 7.58 GN/m3 while for same level of doping processed with the Pulverisette-4 processed material was 6.90 GN/m3. The irreversibility field (Hirr) was 8.50 T for the 5 at.% doped MgB2, while for Pulverisette-4 was 7.11 T.

Study of the Pitting Corrosion under Insulation of Duplex Stainless Steels: Khalil Alahmadi[1]; *Joanna Groza*[1]; [1]UC-Davis

Duplex Stainless Steel (DSS) is a class of stainless steel that has two-phase structure, namely, ferrite (α) and austenite (γ) with around equal amounts of the two phases. DSS offers an attractive combination of mechanical properties and corrosion resistance. Corrosion under insulation (CUI) of this material has not been discussed thoroughly in the past as per the author's knowledge. This paper discusses the CUI (particularly the pitting CUI) of two grades of this material, namely, 2205 and 2507 at different temperatures. Further, results and conclusions will be fully available by the time of the subject meeting.

Study on a New Process for Recovery Rhenium and Producing Ammonium Rhenium from Reduction Solution of Process Copper Smelting: Bai Meng[1]; *Zhan Jing*[1]; Zhang Chuanfu[1]; Wu Jianhui[1]; Fan Youqi[1]; [1]Central South University

Rhenium is a kind of rare metal with its content in the earth shell only at about 7 ×10 - 8 %, so it is very meaningful to recover it. The paper describes distribution of rhenium in copper concentrate ore during the process of copper smelting. Aiming at particularity of reduction solution with peracid, high concentration of arsenic, more impurity and low content of rhenium and problem of avoiding changing property of reduction solution during recovery of ammonium rhenium, a new process for recovery of rhenium and producing ammonium rhenium from reduction solution of process copper smelting, namely, solvent extraction- strip extraction-purification-crystallization. The process has low operation cost and high economic efficiency. Percentage extraction and stripextraction of rhenium are more than 98%. Direct recovery of rhenium is more than 85% and grade of ammonium rhenium product is more than 99%.

Study on Effects of Cement Additives on Properties of Cement by Using the Calorimeter Method: *Daowu Yang*[1]; Chengfeng Wang[1]; Zhongliang Xiao[1]; [1]Changsha University of Science and Techonology

In this paper the used technique to study affect of cement additions on properties of cement was conduction calorimeter. The affect of cement added to one of the three additions (lignosulfonate, citric acid, DBS) and the cement added to all on the pure cement was measured using the TAM Air calorimeter instrument which owns eight channels made by Sweden. And eight curves of heat dissipation of cement hydration was determined. The value of heat dissipation of hydration and the hydration rate was get from the curves. And the affect of additions on the cement was analyzed. Result shows that: the chemical additions such as water reducer(lignosulfonate), set retarder(citric acid) can decrease the value of cement hydration and the increasing temperature differently, also it can delay the time when the curve of heat dissipation appears. Air training admixture DBS affect the heat of hydration and the increasing temperature little.

Study on Electric Conductivity of AlCl3/Benzyltrimethylammonium Chloride Room Temperature Ionic Liquids: Liu Quan[1]; Liu Kui-ren[1]; Han Qing[1]; Tu Gan-feng[1]; [1]Northeasten University

This paper studied influences of organic solvents (ethanol, acetone, ethyl acetate, tetrahydrofuran, toluene and benzene), composition and temperature on electric conductivity of Benzyltrimethylammonium Chloride and anhydrous aluminum chloride (TMBAC/AlCl3) ionic liquids, optimized the aluminum reduction process and characterized Al deposition prepared by using the methods of SEM, XRD and EIS. Except that benzene could significantly improve the electric conductivity, the other solvents were detrimental to this system. The electric conductivity of ionic liquids increased with increasing benzene concentration, and when the concentration of benzene was 50%(vol.), the electric conductivity reached the maximum. The relation curves between temperature and electric conductivity were found to obey Arrhenius equation in the lower temperature range. In the TMBAC/AlCl3 ionic liquids with benzene concentration 50% (vol.), silvery aluminum deposition with dense surface was prepared and had a excellent corrosion resistance.

Study on Phosphorus Recovery from Rare Earth Minerals Containing Apatite by Citric Acid Coordination: Bian Xue[1]; *Wu Wenyuan*[1]; [1]Northeast University

Phosphorus is intergeneration and unreplacement resource. The phosphorus minerals will dry up in middle period of this century in world. The recovery of phosphorus from rare earth minerals containing apatite is meaningful. In this paper, the coordination of citric acid (H3cit) is used to recover phosphorus and separate it with rare earth using the coordination of citric acid. The relationship among the ratio of phosphorus recovery, citric acid addition, pH, temperature, and time was studied, and then the regression equation was obtained. The optimum process conditions of phosphorus recovery were obtained as follows: citric acid concentration 0.05mol•L-1, pH=9, and time 20min, the ratio phosphorus recovery 99.8%, rare earth loss 0.98%. This research gives the support to recover phosphorus from rare earth minerals containing apatite.

Study on the Surface Filming of Magnetic Modified Carbon Fiber: *Xiaozhong Huang*[1]; Zuojuan Du[1]; [1]Central South University

In this paper, the surface filming of the carbon fiber for iron Sol was studied. IR analysis of the iron Sol showed that there are a large number of hydroxyl, carboxyl and other organic groups in the iron Sol, which implies a good infiltration with carbon fiber. The unglued process of the carbon fiber and the heat treatment technology of carbon fiber coating iron Sol were investigated. The carbon fibers are unglued under the protection of N2 and 800°C temperature. The analysis of DTA showed that the heat treatment technology of carbon fiber coating iron Sol is divided into two stages: the first stage of temperature control in the 120°C and the second phase of temperature control in the 300°C. The magnetic modified carbon fibers were prepared by coating thin and uniform iron Sol.

Surface Modification of a Biometallic Aisi 316l Stainless Steel by Means of Pulsed Electron Beam Treatment: *Kemin Zhang*[1]; [1]Shanghai University of Engineering Science

Low energy high current pulsed electron beam (LEHCPEB) is a fairly new technique for surface modifications. The pulsed electron irradiation induces (i) very rapid heating, melting, solidification and cooling of the surface together with (ii) the formation of thermal stress waves. As a result, improved surface properties of the material, often unattainable with conventional surface treatment techniques, can be obtained fairly easily. This is particularly true for corrosion and tribological properties. In the present work, LEHCPEB was applied on two kinds of bio-metallic materials, 316L stainless steel and Ni(50.6 at%)Ti alloy. It was demonstrated that the corrosion resistance and the biocompatibility of the two alloys were significantly improved after the LEHCPEB treatment. The improvement in properties can be attributed to the microstructure and chemical modifications in surface layers induced by LEHCPEB.

Surface Modification of Ti6Al4V Alloy by Pack Boriding: Erdem Atar[1]; Eyup Kayali[2]; *Huseyin Cimenoglu*[2]; [1]Gebze Institute of Technology; [2]Istanbul Technical University

Titanium and its alloys have been widely used in aerospace, chemical and biomedical industries because of their low density, high dynamic and static strengths and excellent corrosion resistance. However, they suffer from poor tribological performance especially when used in wear related engineering applications. In fact poor wear resistance is inherent charcteristics of titanium alloys and can only be improved by surface treatment. In the present study surface hardening of an extensively used Ti6Al4V alloy through boriding was investigated. Boride layer composed of TiB and TiB2 phases were formed on the surface by using pack boriding technique. The hardness of the boride layer was over 2000 HV and caused considerable improvement wear resistance.

Surface Rumpling of Pt-Modified Aluminide Coating with the Thickness of the Pre-Deposited Pt during Fabrication: *Seokjun Hong*[1]; Yongnam Ko[1]; Sunggoon Kang[1]; [1]Hanyang University

Pt-modified aluminide coatings were prepared with various thicknesses of pre-deposited Pt on CM247LC by heat treatment and low-activity high-temperature (LAHT) pack auminizing. After heat treatment, thicknesses of interdiffused area

were individually different with thicknesses of pre-deposited Pt. Also, thicknesses of pre-deposited Pt affected the surface roughening. When the Pt atom and the Ni atom were interdiffused each other, surface morphology was affected because of internal stress and the differential atomic radiuses. After pack auminizing, Pt-modified aluminide coating consisted of a two-phase, a one-phase and an interdiffusion layer. The two-phase layer was increased with increasing thickness of pre-deposited Pt. Also, from 2 to 8 μm, surface roughness was increased with increasing thickness of pre-deposited Pt. However, surface roughness of Pt-modified aluminide coating which was fabricated with pre-deposited Pt of 12 μm was relieved because of crowded $PtAl_2$ phase nearby the coating surface.

Synthesis and Characterization of Novel Biomaterials: *Nikhil Dhawan*[1]; [1]Punjab Engineering College

Biomaterials are widely used in the field of medical science as prosthetics. Metallic biomaterials, in spite of good mechanical properties, suffer from poor corrosion resistance as well as release of toxic elements in the body and cause implant failure, inflammation and body allergies. This problem has been overcome by coating their surface with ceramic biomaterials. The present work deals with some newly synthesized bioactive materials like Hydroxyapatite and Ca-P bioactive glass. HAp and HAp- Bioactive glass composite has been synthesized through powder metallurgy technique and has been characterized for their structure and phase composition using XRD and SEM techniques. Also corrosion resistance has been tested in vitro keeping the biomaterials in simulated body fluids at body temperature. It is expected that these materials, apart from being non- toxic, will exhibit better bonding characteristics to bone tissue.

Synthesis of Meso-Porous CaCO3 Particles by a Spray Drying Method: *Hee Dong Jang*[1]; Kuk Cho[1]; Hankwon Chang[1]; Kikuo Okuyama[2]; [1]Korea Institute of Geoscience & Mineral Resources; [2]Hiroshima University

Synthesis of nanostructured spherical CaCO3 particles having mesopores was investigated using a spray drying method with colloidal suspension of CaCO3 nanoparticles. The CaCO3 nanoparticles ranged from 20 nm to 100 nm in primary particle size were prepared from 3 μm of the particles by ultrafine grinding using a bead mill. Average particle size of the synthesized porous particles was around 1 μm in diameter. The porous CaCO3 particles showed pore size distribution consisting of mesopores ranged from 2 nm to 30 nm. As the primary particle size of CaCO3 nanoparticles increased, mesopores size increased due to a reduction in packing rates of primary CaCO3 nanoparticles composing the walls of nanostructured porous particles. As the surfactant concentration increased in the colloid, smoother surface particles were prpeared but major diameter of mesopores decreased. Mesopores of the particles disappreared when the furnace temperature was higher than 400°C.

The Analog Simulation of Three-Layer Electrolysis Cell for Refining of Aluminum: *Hengchao Zhao*[1]; Huimin Lu[1]; [1]Beijing University of Aeronautics and Astronautics

In the paper, the commercial simulation software ANSYS is used to build the three-dimensional model of refining aluminum cell. According to the relative parameters of the existing 85kA three-layer electrolysis cells as well as reasonable boundary condition hypotheses, the analog simulation computations to electric, temperature and magnetic fields in different production time are carried on, their results tally well with this actual production situation. The feasibility and the accuracy are confirmed in applying these models to analog simulation in the existing cells. Then, using the multiple elements and multiple properties of ANSYS software, the responsibility of 100kA three-layer electrolysis cells for refining aluminum is also checked.

The Annealing and Aging Effect on Irradiated ZnO:Al Film by Cs-137: Meliha Tekin[1]; Eyup Kayali[1]; Huseyin Cimenoglu[1]; *Nilgun Baydogan*[1]; Hande Sengel[2]; Fehiman Akmaz[2]; Ates Parlar[2]; [1]Istanbul Technical University; [2]Sisecam

ZnO:Al thin film was prepared using spin coating technique. Annealing effect on ZnO:Al thin film was evaluated at different temperatures. Annealing temperature was effected the structure of ZnO:Al film. For the determination of aging effect of sun on ZnO:Al film, the ultraviolet light source with double beam was used. The beams of UV light source have at 366 nm as long wave UV light and at 254 nm as short wave UV light. Besides, Cs-137 radioisotope with 9.5 μCi activity was used to accelarate the aging effect on ZnO:Al thin film. Cs-137 with 662 KeV photon energy was an appropriate source to decrease the aging time. Therefore it can be possible to compare the changes of the optical properties after the irradiation of ZnO:Al thin film with a UV light photons and with gamma rays.

The Effect of Sintering Temperature and Pinning Elements on the Superconducting Properties of Spark Plasma Sintered MgB2: *In Shup Ahn*[1]; Su Gun Lim[1]; Dong Woong Kim[1]; Deuk Kyun Kang[1]; [1]Gyeongsang University

Many researches on the MgB2 have been carried out because of high critical temperature(Tc) and current density. In this study, the Mg and B powders of equivalent composition of MgB2 and pinning element of carbon were mixed or milled for 9 hours maximum at argon atmosphere. The MgB2 bulk was fabricated at the various temperatures by Spark Plasma Sintering. The formation of MgB2 phase was confirmed at the temperature of 550°, and the formation temperature decreased to 350° in case of milled powder for 9hours. The relative density of sintered MgB2 was over 99%, which increased as the sintering temperature increases. The densification was proceeded with solid phase and liquid phase sintering behavior step by step without abnormal grain growth. In the PPMS result, the Tc was about 37K in case of carbon pinning element addition. The MgB2 grains size effect on the Tc change was not obtained.

The Effect of Temperature on In-Situ Intrinsic Stress Behavior in Cu Thin Films: *Moohyun Cho*[1]; Sang Ryu[1]; Youngman Kim[1]; [1]Chonnam National University

The intrinsic stress in thin film evolves during nucleation and growth of atoms on the substrate. Cu thin films, which grow in Volmer-Weber type, have unique stress behavior of three stages, such as initial compressive, tensile and incremental compressive. The tensile stress evolution was reported from the volume contraction though island coalescence. The mechanism of compressive stress is still in controversy even though extensive research efforts are being made. Incremental compressive stress may be related to the mobility of adatom on the substrate. To control the mobility of depositing Cu atoms, the substrate temperatures are changed from room temperature to 250° during depositon. We observed the in-situ stresses behavior of Cu thin films during deposition using multi-beam curvature measurement system attached to a thermal evaporation device. When temperature of substrate increased, the thickness at tensile maximum and the slop of incremental compressive stress showed a tendency to decrease.

The Effect over Capacitance Properties of Surfactants Used in Mn(NO3)2 Impregnation Process in High Charge Tantalum Powders: Juan Torres-Castañón[1]; *Miguel Esquivel-Aguirre*[1]; Héctor Barrientos[1]; Ana Pimentel[1]; Cristina Mota-Caetano[1]; Juan Pérez-Medina[1]; [1]Kemet De Mexico

The manganese dioxide has been used since several years ago like a counter electrode in the tantalum capacitor fabrication. It has been reported that the additions of surfactants reduce the interfacial tension (liquid/solid interface) and help to improve the impregnation process. The impregnation with a non-ionic surfactant in tantalum pellets made from high CV powders was investigated at 30-60ºC and concentrations of 0,01-0,1% wt. The influence of the surfactant in the MnO2 structure was electrically characterized and phase distribution was analyzed with Scanning Electron Microscopy. A recovery in capacitance (~10%) was detected for under treatment part types with 100 and 320 μF. The surfactant concentration into the solution is the main factor for the capacitance recovery and the electrical performance. The best capacitance recovery and electrical performance was obtained with 0.05% wt. of surfactant.

The Effects of Finish Cooling Temperature on Yield Strength 800MPa Heavy Steel Plate Subjected to Direct Quenching Process: *LianDeng Yao*[1]; Sixin Zhao[1]; Xiaoting Zhao[1]; Hongbin Li[1]; [1]Baosteel Technology Center

A kind of low carbon micro-alloyed heavy steel plates with thickness 40mm and low susceptibility to welding crack which yield strength exceed 800MPa, tensile strength exceed 950MPa, -40ºC; charpy V-notch impact energy exceed 120J was produced by direct quenching process. The structure constitutions of heavy plates are bainitic ferrite plates which thickness less than 1μm and M/A constitute decorating at bainitic plates boundaries. Bainitic ferrite plates composed by sub-plate become thinner with the finish cooling temperature decreasing. The charpy V-notch impact energy at -40ºC; of the plate direct quenching to 350ºC; is lower than that direct quenching to room temperature buy higher than that direct quenching to 250°C. Bainitic ferrite plate of experimental steel plates with various finish cooling temperature have high density dislocation. The bainite nucleation and growth process of experimental steel can be explained reasonably by diffusional mechanism.

The Effects of Probe Diameter on Optimum FSW Conditions of 5456-H116 Alloy for Leisure Ship: *Kim Seong-jong*[1]; Lee Seung-Jun[1]; Han Min-Su[1]; Park Jong-Seek[1]; Park Jae-Cheul[1]; [1]Mokpo Maritime University

This investigated the optimum FSW conditions of 5456-H116 alloy for leisure ship. Moreover, in probe diameter of 6mm with 15mm/min, the rough surface and

void with insufficiency of heat input due to low rotation speed were observed at 170-210RPM. However, a lot of chip due to excessive heat input is observed in 1100-2500RPM. In addition, the effect of heat input is prominently presented at the bottom side. In 15mm/min increased with the increasing of rotation speed due to heat input increase by increasing friction. The mechanical characteristics are decreased by accelerating softening of base metal due to increasing of heat input. Acknowledge: This research was financially supported by MOCIE and KOTEF through the Human Resource Training Project for Regional Innovation.

The Electrochemical Leaching of the Chalcopyrite Concentrate in Acid Solution: *Izolda kakhniashvili*[1]; Archil Benashvili[1]; [1]R.Agladze Institut of Inorganic Chemistry and Electrochemistry

The anodic dissolution of the suspension electrode made of Madneuli chalcopyrite concentrate in 30 gl-1 H2SO4 solution was investigated using platinum and chalcopyrite probes. The experimental results suggest that the anodic dissolution of the chalcopyrite suspension electrode occurs not only when the electrode comes into contact with the current fidder but also in solution.The anodic oxidations of chalcopyrite concentrate proceeds in acidic solution in the presence of NaCl. It was established the optimal parameters of the processes.

The Evaluation of Densified Layer Formation Mechanism and Thickness during Dry Sliding Wear of Porous Powder Metallurgy Steels: *Shaahin Amini*[1]; Kavan Hazeli[2]; [1]University of California, Riverside; [2]Iran Test and Research Auto Company (ITRAC)

When a porous powder metallurgy part is worn by a counterbody, intense shear stresses are exerted on the surface and subsurface owing to the both normal load and tangential load (i.e. friction). Hence, the pores near the surface are closed owing to intense plastic deformation in this area and a hardened densified layer is formed. This densified layer has the thickness in which applied stresses are more than the yield stress of the matrix. In this research a porous Distaloy AE material which is a partially alloyed steel powder was worn by AISI 52100 steel in a reciprocating manner. Then subsurface stresses derived from normal and tangential load were calculated. The thickness of densified layer was obtained by comparing these stresses with yield stress of the matrix. The results compare with the metallographic photos and the differences are discussed.

The Investigation of Microstructural Changes in ZnO:Al Thin Film by Beta Irradiation: Hande Tugral[1]; Huseyin Cimenoglu[1]; *Nilgun Baydogan*[1]; Hande Sengel[2]; Fehiman Akmaz[2]; Ates Parlar[2]; [1]Istanbul Technical University; [2]Sisecam

ZnO:Al thin film was prepared using spin coating technique. After the coating process the texure of ZnO:Al film was exposed to Sr-90 radioisotope. It was found that the texure of the film can be affected with beta radiation. The microstructural changes using Sr-90 is critical with the charge trapping of radiolytic electrons or holes and the formation of defect centers and radiolytic electrons or holes. Beta radiation at ZnO:Al film led to a change in the physical properties such as colour when the beta radiation penetrated into the film. The evaluation of colour changes of irradiated ZnO:Al film is possible using the colour system. The changes of dominant wavelength, brightness and excitation purity of ZnO:Al transparent film were evaluated. Colour co-ordinates were used for the determination of dominant wavelength and excitation purity of ZnO:Al thin film in the CIE tristimulus system.

The Microstructure and Mechanical Properties of As-HIP FGH 95 P/M Superalloy for High Pressure Turbine Blade Retainers: *Yu Tao*[1]; Jian Jia[1]; Jiantao Liu[1]; Yiwen Zhang[1]; [1]CISRI

FGH 95 is a powder metallurgy (P/M) processed superalloy, which was developed in the 1980s in China. One of the applications of FGH 95 is for high pressure turbine blade retainers. The manufacturing processes used to produce FGH 95 blade retainers consist of atomization by plasma rotating electrode process (PREP), hot isostatic pressing (HIP) and a heat treatment with sub-solvus solution. The material has a equiaxed grain structure (about ASTM 7) with a fine dispersion of gamma prime and carbide precipitates. Batch production statistics of the mechanical properties for FGH 95 blade retainers were investigated. The as-HIP FGH95 blade retainers show high strength in room temperature and 650°, excellent creep resistance and stress rupture strength in 650°.

The Reheating Behavior and Extrudability of Al-Zn-Mg Alloy Billet with Added Scandium: *Sung-Yong Shim*[1]; Dae-Hawn Kim[1]; In-Sub Ahn[1]; Su-Gun Lim[1]; [1]Gyeonsang National University

The grain growth behavior under reheating process and extrudability of Al-Zn-Mg-(Sc) alloy fabricated by cooling plate method were evaluated. When Sc was added in aluminum alloy, the formed Al_3Sc precipitation performed grain-boundary pinning, which enabled the reheating process for Thixo-extrusion to reduce the grain growth. With the addition of Sc, the reheating behavior of the Al-Zn-Mg alloy was observed by optical microscope and EMPA after being heated to solid-liquid temperatures. The extrudability was evaluated by examining the surface cracking under extrusion conditions such as ram speed, billet heating temperature and extrusion ratio. The grain growth was significantly reduced when the Sc content exceeded 0.1 wt.% and the grain size of the Al-Zn-Mg+0.1wt.%Sc alloy was maintained at about 70° after 30 minutes at 600°. The extrudability was superior to that of conventional billets because the semi-solid materials have the advantage of having a low shear stress that allows deformation.

The Role of Iron Addition on the Fire Assay of Pyritic Ores: *Ahmet Turan*[1]; Hakan Morcali[1]; Onuralp Yucel[1]; [1]Istanbul Technical University

Fire assay is the most reliable and essential method which is employed to accurately analyse the precious metal content of ores. The avoiding from lead containing matte formation is the necessity for the fire assay of pyritic ores. Therefore iron is added on the smelting stage of pyritic ores in order to reduce lead from matte. In this study, experiments were conducted to understand the effects of different quantities of additional iron on the gold and silver recovery from pyritic ores. Specimens were fused by using fluxes and PbO, which accumulates precious metals, with various quantities of iron. AAS was used to analyze the precious metals obtained. Correlation between the quantity of additional iron and the recovery of gold and silver was investigated.

The Shock Wave in High Velocity Compaction of Iron Powders: *Haiqing Yin*[1]; Xuanhui Qu[1]; Shengyu Zhou[1]; Jianzhong Wang[1]; Mingjun Yi[1]; Sharon Elder[2]; [1]University of Science and Technology Beijing; [2]Pennsylvania State University

High velocity compaction of iron powder in both single impact and multiple impacts was investigated. The shock wave of the impact force and the green density were studied. The shock wave showed the characteristics of shock wave discontinuity during compaction. The shock wave of the initial impact was observed as saw-tooth waves. The compaction velocity and density prior to compaction were key factors affecting value and shape of the shock wave. With the increase of the compaction velocity, the working duration of the initial impact on the powder shortened. And the secondary wave on the initial wave became steeper with a greater peak force on the powder. Further, the saw-tooth shape of the shock wave disappeared with the increasing density prior to the last impact in double and triple impacts. In double impacts, the green density was found to be greater than those in single and triple impacts.

The Thermal Decomposition Behaviour of Ammonium Heptamolybdate Tetrahidrate: *Kemal Can Kevser*[1]; Aliye Arabaci[1]; Ibrahim Yusufoglu[1]; [1]University of Istanbul

In this study, the thermal decomposition of ammonium heptamolybdate tetrahydrate (AHM) in different heating rates and under different air and nitrogen gas flow rates was investigated. Therefore, analysis techniques like TGA, DTA and EGA were used. In the thermal decomposition of AHM three well-defined steps were observed and the intermediate and final products of each decomposition step were characterized by using XRD and FTIR analysis techniques and their morphologies were determined by SEM analysis. The characterization of the products and thermogravimetric analyses showed that AHM decomposes as (NH4)6Mo7O24·4H2O · (NH4)4Mo5O17 + (NH4)2Mo2O7 · (NH4)2Mo4O13 · MoO3 in air and as (NH4)6Mo7O24·4H2O · (NH4)4Mo5O17 + (NH4)2Mo2O7 · (NH4)2Mo4O13 · MoO3-x in nitrogen gas. The activation energy values were calculated in air and nitrogen gas atmospheres for the each decomposition step observed in TGA diagrams by applying Ozawa method.

Theoretical Investigation of Sulfur Adsorption on Fe (100): *Weimin Cao*[1]; Anna Delin[1]; Taishi Matsushita[1]; Seshadri Seetharaman[1]; [1]Royal Institute of Technology (KTH)

Electronic and structural properties of the atomic sulfur adsorbed on the iron surface (100) are examined by using the density functional theory (DFT). The sulfur coverage is considered from a quarter to two monolayers (MLs). The adsorption energy and work function are calculated for three different adsorption sites of sulfur. The calculated results indicate that the most likely site for S adsorption is the hollow site on Fe (100), which is agreement with experiment. In addition, the work function increased after the S adsorption on the Fe (100) surface, which implies the charge transfer from the surface to sulfur. The present results are in agreement with the other theory calculations.

Thermodynamic Study on Complex System Co (II)-C2O42—NH3 -NH4+-H2O for Preparation of Fibrous Cobalt Powder Precursor: *Zhan Jing*[1]; Zhang Chuanfu[1]; Wu Jianhui[1]; Yang Ping[1]; [1]Central South University

Based on the principles of simultaneous equilibrium and mass balance, a series of thermodynamic equilibrium equations of Co(II)-C2O42—NH3-NH4+-H2O system at ambient temperature are deduced theoretically and the logarithm concentration versus pH (logc-pH) diagrams at different solution compositions are drawn. The results show that when pH is above 8.0, cobalt ions coordinate with ammonia and the precipitation proceeds slowly accompanying with the release of cobalt ions from the multicoordinated Co(NH3)n2+(n=1, 2,…, 6), the morphology of cobalt powder precursor is fibrous; when pH is below 8.0, cobalt ions directly react with C2O42-, the morphology of cobalt powder precursor is cubic-shape. According to thermodynamics analysis and calculation, some experiments were done to validate the relation between the total concentration of cobalt ions and pH in this study.

Ti-6Al-4V Alloy for Tooling Applications in Semi-Solid Processing: Kemal Korkmaz[1]; *Yücel Birol*[1]; [1]TÜBITAK-Marmara Research Center

The processing of metals in the semi-solid state offers the opportunity of manufacturing complex structural parts in near-net shape. The process temperatures are usually in the semi solid area of metals, thus it is possible to decrease cost and save energy. However, tool dies for semi-solid forming are subjected to extreme conditions and life time of the tool dies is restricted by thermo-mechanical load cycles. The purpose of the present study is to investigate Ti-6Al-4V alloy as tool die materials. In this study, a ceramic layer is formed on Ti-6Al-4V alloy by micro-arc oxidation (MAO) in solutions of Na3PO4 and NaAlO2. MAO is mainly promising a new surface technology for Ti-6Al-4V alloys, where thick and hard ceramic oxide layers can be formed. After MAO process, the wear, heat and corrosion resistance of these alloys can significantly be improved.

Tin Recovery from Printed Circuit Boards of Obsolete Computers Using a Hydrometallurgical Approach: *Afonso Martins*[1]; [1]Universidade Federal de Minas Gerais

This paper presents the preliminary experimental results for leaching of printed circuit boards from obsolete computers aiming at extraction of tin and recovery it by precipitation. Printed circuit boards were dissembled, cut off in small pieces and fed into a cylinder mill. The powder obtained was leached using aqueous solutions 2,18N H2SO4, 2,18N H2SO4+3,0N HCl, 3,0N HCl or 3,0N HCl+1,0N HNO3. The lowest values for percent of extraction were obtained for the 2,18N H2SO4 (2.7% Sn). Meanwhile, the leach system 3,0N HCl+1,0N HNO3 exhibited 98% Sn.Precipitates were obtained at different pH values by neutralization of the leach liquors using NaOH. The leach system 3,0N HCl+1,0N HNO3 presented the highest recovery values from the powder feed (84.1% Sn) and from the leach liquor (85.8% Sn).

Titanium Extraction by Electrochemical Reduction of TiO2: *Chaganti Nagesh*[1]; [1]DMRL

Titanium extraction by electrochemical reduction of titanium dioxide (TiO2)is emerging as a potential alternate for titanium sponge production, owing to its several advantages resulting in cost and energy savings. In this work, the electrochemical reduction process has been studied on a laboratory scale of 100-200 grams per batch. Experimental work involving conversion of titanium dioxide granules into titanium metal by subjecting them to a cathodic treatment in a molten calcium chloride bath at a temperature of 950C, and using graphite anode. After the experiment, the sponge granules are thoroughly washed with water, acetic acide and dilute HCl. Excellent metallization has been found in granules which was confirmed by metallurgical characterization techniques viz. metallography, SEM, EDAX, EPMA etc. Attempts have also been made to evolve a theoretical kinetic model that describes the metallization process during the electrochemical reduction.

Titanium Sponge Production in India: *Chaganti Nagesh*[1]; Brahmendra Kumar Gummadi[1]; Sitaraman TS[1]; Ramachandran CS[1]; [1]DMRL

India possesses large and rich reserves of ilmenite (FeOTiO2), an important mineral of titanium. Defence Metallurgical Research Laboratory, Hyderabad, India (DMRL) has successfully developed the technology for production of titanium sponge by high temperature magnesium reduction of pure titanium tetrachloride followed by vacuum distillation of reduced mass employing a 'Combination unit'. This development work includes (i) development of distillation columns for TiCl4 purification, (ii) design, development and operation of equipment for conducting Reduction and Vacuumd distillation processes in a batch size of 3000 kg of sponge and (iii) development of equipment and tooling for titanium sponge grading, cutting and quality evaluation to prepare homogenous lots of high quality sponge. This paper brings out salient features of DMRL technology and results of the technology development program including the improved understanding of the metal production process. Tthe country's first commercial titanum sponge plant is coming up with this technology.

Toolcoatings as Thermocouple for Chipping: *Klaus Pantke*[1]; Heilmann Markus[1]; Dirk Biermann[1]; [1]University of Dortmund

The acknowledgement of temperature influences onto the cutting edge and workpieces achieves a growing relevance. Particularly with regards to the cutting material-, coating-, and cooling lubricant selection, the knowledge of appearing temperatures is essential. Up to now, the action-close thermo measurement at the cutting edge is conducted by video-thermographic recordings, pyrometers or according to the principle of resistance-measurements. Modern coating technology offers new options. Already established measuring methods allow the detection of temperature and wear following the principle of conductivity variation by close meshed conductor structures plated on the cutting inserts. An improved method utilizing an alternative physical principle now allows to implicate coatings for temperature measurements by means of the so-called "Seebeck-Effect". Applying the principle of thermo electricity just as in conventional thermo couples, different metals are affiliated with each other and exposed to an temperature gradient, so that a measurable voltage results.

Two-Step Sintering of Nd-Fe-B Powder: *Se Hoon Kim*[1]; Hoon Sup Kim[1]; Min Suh Park[1]; Ji Hoon Seo[1]; Young Do Kim[1]; [1]Hanyang University

Sintered Nd-Fe-B magnets have been wildly used due to their excellent magnetic properties. However, heterogeneous microstructure of Nd-Fe-B magnet is an important factor limiting their magnetic property. Therefore, modifying a sintering process has been an important method for better homogeneous microstructure. In this study, Nd-Fe-B powder was fabricated by strip-casting and jet milling. The powder was compacted in a magnetic field. After that, the green compact was sintered at temperature between 1050°C and 1150°C as first-step, then, second-step was sintered at temperature between 900°C and 1000°C. Two-step process was employed for the sintering of Nd-Fe-B powder to obtain homogeneous grain size in bulk part. Densification over 99% could be obtained by the two-step sintering of Nd-Fe-B powder with 5 μm in Nd2Fe14B phase and the Nd-rich phase was homogeneously distributed. Moreover, the two-step sintering process led to uniform grain size distribution with the improvement of magnetic properties.

Uniform Depth of Cladding through Vision-Based Monitoring of VP GTAW Cladding of Aluminum Alloys: *Rouzbeh Sarrafi*[1]; [1]Southern Methodist University

Variable-polarity GTAW (VP-GTAW) process is capable of producing sound clads on aluminum alloys due to the real-time removal of oxide layers. However, heat accumulation in the workpiece during the cladding causes non-uniform depth of clads, making heat management a big challenge to the application of VP-GTAW for cladding of aluminum alloys. In this research, a machine-vision system was integrated to monitor the molten pool width during cladding. The image of the bright arc plasma has been almost eliminated by an illumination/filtering technique. A low-resolution CCD camera was used to capture the images in real-time. The results showed that by this method, clear images of the molten pool boundary are obtained so that they can be subsequently integrated to a control system. In addition, it is experimentally shown that by controlling the width of molten pool by altering current or travel speed, a uniform depth of clad can be achieved.

Upgrading Titaniferous Metallurgical Slag by Activation -Acid Leaching Process: *Tao Jiang*[1]; Haigang Dong[1]; Yufeng Guo[1]; Guanghui Li[1]; Yongbin Yang[1]; [1]Central South University

Large reserve of vanadium-titanium magnetite ore has been found in China. Currently, Ilmenite concentrate with 47%TiO2 has been obtained from the ore by beneficiation. By electrical furnace smelting, the concentrate is processed into the titanium-rich slag with 73% TiO2, which is still not suitable for the production of titanium white by chlorination process due to its high content of impurities, such as CaO, MgO, etc. This work has developed a new process to upgrade the slag. The slag is first activated by roasting at a temperature of 700°C to 900°C with addition of alkali metal salts. The activated slag is then leached by sulphuric acid and the leached slag is calcined at a temperature of 900°C. By this process, the Ti-rich product with 92% TiO2 is obtained. The mechanism of activation-acid leaching is studied by XRD analysis and thermodynamic investigation.