TMS2007

136th Annual Meeting & Exhibition

Linking Science and Technology for Global Solutions

Technical Program

ROOM	Monday		Tuesday		Wednesday		Thursday
	AM	PM	AM	PM	AM	PM	AM
America's Seminar	Materials Processing under the Influence of External Fields: Session I	Materials Processing under the Influence of External Fields: Session II	Intellectual Property in Materials Science: Patents, Tech Transfer and Licensing: Patents	Intellectual Property in Materials Science: Patents, Tech Transfer and Licensing: Commercialization	Materials Processing under the Influence of External Fields: Session III	Materials Processing under the Influence of External Fields: Session IV	Materials Processing under the Influence of External Fields: Session V
Asia 1	Bulk Metallic Glasses IV: Glass Science and Technology	Bulk Metallic Glasses IV: Mechanical Properties I	Bulk Metallic Glasses IV: Alloy Development and Glass-Forming Ability	Bulk Metallic Glasses IV: Mechanical Properties II	Bulk Metallic Glasses IV: Supercooled Liquids and Crystallization	Bulk Metallic Glasses IV: Mechanical Properties III	Bulk Metallic Glasses IV: Mechanical Properties IV
Asia 2	Materials in Clean Power Systems II: Fuel Cells, Solar, and Hydrogen-Based Technologies: Plenary Session	Materials in Clean Power Systems II: Fuel Cells, Solar, and Hydrogen-Based Technologies: PEMFCs	Materials in Clean Power Systems II: Fuel Cells, Solar, and Hydrogen-Based Technologies: SOFCs I	Materials in Clean Power Systems II: Fuel Cells, Solar, and Hydrogen-Based Technologies: SOFCs II	Materials in Clean Power Systems II: Fuel Cells, Solar, and Hydrogen-Based Technologies: Materials Oxidation/ Corrosion and Protection	Materials in Clean Power Systems II: Fuel Cells, Solar, and Hydrogen-Based Technologies: Materials for Clean Coal Power Generation and Gas Separation	Materials in Clean Power Systems II: Fuel Cells, Solar, and Hydrogen-Based Technologies: Materials for Solar Cells and Photovoltaic Systems
Asia 3	Innovations in Titanium Technology Symposium: Low Cost Materials and Processing	Innovations in Titanium Technology Symposium: Novel Materials and Processes I	Innovations in Titanium Technology Symposium: Novel Materials and Processes II	Innovations in Titanium Technology Symposium: Advances in Materials Processing	Innovations in Titanium Technology Symposium: Advances in Alloy Development	Innovations in Titanium Technology Symposium: Microstructure and Properties I	Innovations in Titanium Technology Symposium: Microstructure and Properties II
Asia 4	Properties and Performance of High Temperature Alloys and Coatings: Single Crystal Alloys I	Properties and Performance of High Temperature Alloys and Coatings: Polycrystalline Alloys	Properties and Performance of High Temperature Alloys and Coatings: Single Crystal Alloys II and Oxidation	Properties and Performance of High Temperature Alloys and Coatings: Coatings and Oxidation I	Properties and Performance of High Temperature Alloys and Coatings: Coatings and Oxidation II	Properties and Performance of High Temperature Alloys and Coatings: Intermetallics and Multidiscipline	
Asia 5	SMD Symposium: Mechanical Behavior of Nanostructured Materials, in Honor of Carl Koch: Fatigue, and Strengthening Mechanisms at Small Length Scale	SMD Symposium: Mechanical Behavior of Nanostructured Materials, in Honor of Carl Koch: Processing and Characterization of Materials Subjected to Severe Plastic Deformation	SMD Symposium: Mechanical Behavior of Nanostructured Materials, in Honor of Carl Koch: Plasticity and Deformation Mechanisms at Small Length Scale I	SMD Symposium: Mechanical Behavior of Nanostructured Materials, in Honor of Carl Koch: Stability, Strain and Stress - and - Poster Sesion: Mechanical Properties of Nanostructured Materials	SMD Symposium: Mechanical Behavior of Nanostructured Materials, in Honor of Carl Koch: Plasticity and Deformation Mechanisms at Small Length Scale II	SMD Symposium: Mechanical Behavior of Nanostructured Materials, in Honor of Carl Koch: Plasticity and Deformation Mechanisms at Small Length Scale III	SMD Symposium: Mechanical Behavior of Nanostructured Materials, in Honor of Carl Koch: Microstructure and Mechanical Properties of Nanostructured Materials
Australia 2	Recycling and Waste Processing: Materials Recovery from Wastes	Recycling and Waste Processing: Batteries and Co/Ni	Recycling and Waste Processing: Automotive Recycling, Global Challenges and Opportunities	Recycling and Waste Processing: Precious Metals Recovery	Recycling and Waste Processing: Aluminum	Recycling and Waste Processing: Other Nonferrous	

Monday		Tuesday		Wednesday		Thursday	ROOM
AM	PM	AM	PM	AM	PM	AM	
Innovations in Measurement Science to Assess the Performance of New Materials in the Real-World: Fundamental Measurement Methods	8th Global Innovations Symposium: Trends in Materials and Manufacturing Technologies for Energy Production: Plenary	Innovations in Measurement Science to Assess the Performance of New Materials in the Real-World: High Strain Rate Deformation	8th Global Innovations Symposium: Trends in Materials and Manufacturing Technologies for Energy Production: Session I	Innovations in Measurement Science to Assess the Performance of New Materials in the Real-World: Characterization of Advanced Materials	Innovations in Measurement Science to Assess the Performance of New Materials in the Real-World: Advanced Measurement Techniques		Australia 3
Advances in Microstructure-Based Modeling and Characterization of Deformation Microstructures: Characterization of Deformed Structures I	Advances in Microstructure-Based Modeling and Characterization of Deformation Microstructures: Modeling of Deformed Structures I	Advances in Microstructure-Based Modeling and Characterization of Deformation Microstructures: Characterization of Deformed Structures II	Advances in Microstructure-Based Modeling and Characterization of Deformation Microstructures: Modeling of Deformed Structures II	Advances in Microstructure-Based Modeling and Characterization of Deformation Microstructures: Modeling of Deformed Structures III	Advances in Microstructure-Based Modeling and Characterization of Deformation Microstructures: Characterization of Deformed Structures III		Europe 1
Diffusion in Advanced Materials and Processing: Atomistic and Multiscale Simulations	Diffusion in Advanced Materials and Processing: Interfaces, Surfaces and Nanostructures	Diffusion in Advanced Materials and Processing: Energy Technology	Diffusion in Advanced Materials and Processing: Materials Processing	Diffusion in Advanced Materials and Processing: Phenomenology and Experiments	Diffusion in Advanced Materials and Processing: Intermetallics and Glasses		Europe 2
Dynamic Behavior of Materials: Deformation I	Dynamic Behavior of Materials: Deformation II	Dynamic Behavior of Materials: Deformation III	Dynamic Behavior of Materials: Deformation IV	Dynamic Behavior of Materials: Mechanical Properties I	Dynamic Behavior of Materials: Mechanical Properties II	Dynamic Behavior of Materials: Fracture	Europe 3
Biological Materials Science: Bioinspired Materials	Biological Materials Science: Mechanical Behavior of Biomaterials	Biological Materials Science: Biological Materials I	Biological Materials Science: Biological Materials/ Bio-Medical - and - Poster Session	Biological Materials Science: Implant Biomaterials	Biological Materials Science: Functional Biomaterials and Devices	Biological Materials Science: Biological Materials II	Europe 4
Materials Issues for Advanced Nuclear Systems: Energy Generation and Waste Issues	Materials Issues for Advanced Nuclear Systems: Material Characterization Issues	General Abstracts: SMD: Advances in Steel I	General Abstracts: SMD: Advances in Steel II	General Abstracts: SMD: Microstructure and Properties of Materials	General Abstracts: SMD: Nickel Alloys and High Temperature Materials I		Europe 5
Refractory Metals 2007: Processing and Mechanical Deformation	Refractory Metals 2007: Oxidation and Thin Films	Fundamentals of Shape Memory and Related Transitions: Electronic Structure and Phonons	Fundamentals of Shape Memory and Related Transitions: Atomistic and Microstructural Mechanisms	Fundamentals of Shape Memory and Related Transitions: Mechanical Behavior	Fundamentals of Shape Memory and Related Transitions: Multiscale Modeling and Applications	General Abstracts: SMD: Processing and Properties of Light Metals	Europe 6
Advances in Computational Materials Science and Engineering Methods: Methods at the Atom Scale I	Advances in Computational Materials Science and Engineering Methods: Methods at the Atom Scale II	Advances in Computational Materials Science and Engineering Methods: Phase Field Methods I	Advances in Computational Materials Science and Engineering Methods: Phase Field Methods II	Advances in Computational Materials Science and Engineering Methods: Finite Element Method I	Advances in Computational Materials Science and Engineering Methods: Finite Element Method II	Advances in Computational Materials Science and Engineering Methods: Dedicated Computational Methods	Europe 7

ROOM	Monday		Tuesday		Wednesday		Thursday
	AM	PM	AM	PM	AM	PM	AM
Europe 8	Microstructural Processes in Irradiated Materials: Dislocation - Obstacle Interactions and Radiation Induced Segregation	Microstructural Processes in Irradiated Materials: Irradiation Effects in Ceramics	Microstructural Processes in Irradiated Materials: Modeling, Microstructure and Embrittlement in Fe-Cr Alloys	Microstructural Processes in Irradiated Materials: Modeling - and - Poster Session I	Microstructural Processes in Irradiated Materials: Reactor Pressure Vessel Steels	Microstructural Processes in Irradiated Materials: He Effects, Deformation and Fracture - and - Poster Session II	Microstructural Processes in Irradiated Materials: Defect Clusters and Fundamental Radiation Effects
Europe 9	Plasticity from the Atomic Scale to Constitutive Laws: Dislocation Core Structure and Solute-Dislocation Interactions	Plasticity from the Atomic Scale to Constitutive Laws: Dislocation Solute, Precipitate and Grain Boundary Interactions	Plasticity from the Atomic Scale to Constitutive Laws: Atomistic Simulations of Dynamic Processes and Nano-Scale Plasticity	Plasticity from the Atomic Scale to Constitutive Laws: Dislocation Ensembles	Plasticity from the Atomic Scale to Constitutive Laws: Meso-Scale Plasticity	Plasticity from the Atomic Scale to Constitutive Laws: Rate Limiting Behavior and Informed Constitutive Laws	
Europe 10	Advanced Metallic Composites and Alloys for High Performance Applications: Advanced Metallics	Advanced Metallic Composites and Alloys for High Performance Applications: Fe and Ni Alloys and Composites	Advanced Metallic Composites and Alloys for High Performance Applications: Refractory Alloys and Composites	Advanced Metallic Composites and Alloys for High Performance Applications: Al Alloys and Composites	Advanced Metallic Composites and Alloys for High Performance Applications: Ti Alloys and Composites	Advanced Metallic Composites and Alloys for High Performance Applications: Metallic Composites	Computational Thermodynamics and Phase Transformations: Nanomaterials and Confined Systems II
Europe 11	Computational Thermodynamics and Phase Transformations: First Principles and Atomistic Calculations of Phase and Alloy Thermodynamics I	Computational Thermodynamics and Phase Transformations: First Principles and Atomistic Calculations of Phase and Alloy Thermodynamics II	Computational Thermodynamics and Phase Transformations: Microstructure Properties and Evolution I	Computational Thermodynamics and Phase Transformations: Microstructure Properties and Evolution II	Computational Thermodynamics and Phase Transformations: Modeling of Phase Transformations I	Computational Thermodynamics and Phase Transformations: Nanomaterials and Confined Systems I	Computational Thermodynamics and Phase Transformations: Modeling of Phase Transformations II
N. H. Foyer		General Poster Session					
Northern A1	MPMD Symposium: Mechanics and Materials Modeling and Materials Design Methodologies, in the Honor of Dr. Craig Hartley's 40 Years of Contributions to the Field of Mechanics and Materials Science: Microstructure Analysis and Representation I	MPMD Symposium: Mechanics and Materials Modeling and Materials Design Methodologies, in the Honor of Dr. Craig Hartley's 40 Years of Contributions to the Field of Mechanics and Materials Science: Homogenization/ Constitutive Behavior I	MPMD Symposium: Mechanics and Materials Modeling and Materials Design Methodologies, in the Honor of Dr. Craig Hartley's 40 Years of Contributions to the Field of Mechanics and Materials Science: Homogenization/ Constitutive Behavior II	MPMD Symposium: Mechanics and Materials Modeling and Materials Design Methodologies, in the Honor of Dr. Craig Hartley's 40 Years of Contributions to the Field of Mechanics and Materials Science: Materials Design	MPMD Symposium: Mechanics and Materials Modeling and Materials Design Methodologies, in the Honor of Dr. Craig Hartley's 40 Years of Contributions to the Field of Mechanics and Materials Science: Nanostructure, Defects and Properties	MPMD Symposium: Mechanics and Materials Modeling and Materials Design Methodologies, in the Honor of Dr. Craig Hartley's 40 Years of Contributions to the Field of Mechanics and Materials Science: Microstructure Analysis and Representation II	General Abstracts: MPMD: Structure/ Processing/ Properties Relationships
Northern A2	Materials Processing Fundamentals: Solidification and Deformation Processing	Materials Processing Fundamentals: Process Modeling	Materials Processing Fundamentals: Smelting and Refining	Materials Processing Fundamentals: Powders, Composites, Coatings and Measurements	General Abstracts: MPMD: In Situ Synthesis and Rapid Prototyping	General Abstracts: MPMD: Modeling and Simulation of Materials and Processes	General Abstracts: MPMD: Processing and Microstructural Development

Monday		Tuesday		Wednesday		Thursday	ROOM
AM	PM	AM	PM	AM	PM	AM	
Frontiers in Solidification Science: Nucleation and Crystal Structure	Frontiers in Solidification Science: Atomic Scale - and - Poster Session	Frontiers in Solidification Science: Microstructures I	Frontiers in Solidification Science: Microstructures II	Degradation of Light Weight Alloys: Session I	Degradation of Light Weight Alloys: Session II		Northern A3
General Abstracts: MPMD: Forming of Materials and Processes	Aluminum Alloys for Transportation, Packaging, Aerospace and Other Applications: Aluminum Applications	Aluminum Alloys for Transportation, Packaging, Aerospace and Other Applications: Aluminum Products	Aluminum Alloys for Transportation, Packaging, Aerospace and Other Applications: Alloy Development	Aluminum Alloys for Transportation, Packaging, Aerospace and Other Applications: Alloy Processing	Aluminum Alloys for Transportation, Packaging, Aerospace and Other Applications: Alloy Characterization	Aluminum Alloys for Transportation, Packaging, Aerospace and Other Applications: Alloys Mechanical Behavior	Northern A4
General Abstracts: EPD: Hydrometallurgy, Wastewater Treatment	Cast Shop Technology: Cast House Operations and Melting	Cast Shop Technology: Metal Treatment	Cast Shop Technology: Quality Measurements and Grain Refining	Cast Shop Technology: Casting	Cast Shop Technology: Solidification and Microstructure	Cast Shop Technology: Cast Shop Safety	Northern E1
	Shape Casting: The 2nd International Symposium: Liquid Metal/ Solidification	Shape Casting: The 2nd International Symposium: Process Design/Analysis	Shape Casting: The 2nd International Symposium: Structure/Property	Shape Casting: The 2nd International Symposium: Modeling	Shape Casting: The 2nd International Symposium: Applications/ Novel Processes		Northern E2
General Abstracts: EPD: Pyrometallurgy, Base Metals	Friction Stir Welding and Processing IV: Session I	Friction Stir Welding and Processing IV: Session II	Friction Stir Welding and Processing IV: Session III	Friction Stir Welding and Processing IV: Session IV	Friction Stir Welding and Processing IV: Session V	Friction Stir Welding and Processing IV: Session VI	Northern E3
		Alumina and Bauxite: Alumina Refinery Safety and Integrity	Alumina and Bauxite: Alumina Refinery Design and Development	Alumina and Bauxite: Bauxite, Digestion, Red Mud, Byproducts	Alumina and Bauxite: Role of Surface Chemistry in Enhancing Refinery Performances		Northern E4
Pb-Free Electronic Solders: Alloy Design, Characterization and Service Reliability: Interfacial Effects	Pb-Free Electronic Solders: Alloy Design, Characterization and Service Reliability: Microstructure and Characterization	Pb-Free Electronic Solders: Alloy Design, Characterization and Service Reliability: Electromigration and Void Formation	Pb-Free Electronic Solders: Alloy Design, Characterization and Service Reliability: Whisker Growth, Design, and Modeling	Pb-Free Electronic Solders: Alloy Design, Characterization and Service Reliability: Processing and Reliability Issues	Pb-Free Electronic Solders: Alloy Design, Characterization and Service Reliability: Mechanical Characterization		Oceanic 1
Internet and Other Electronic Resources	Phase Stability, Phase Transformations, and Reactive Phase Formation in Electronic Materials VI: Session I	Phase Stability, Phase Transformations, and Reactive Phase Formation in Electronic Materials VI: Session II	Phase Stability, Phase Transformations, and Reactive Phase Formation in Electronic Materials VI: Session III	Phase Stability, Phase Transformations, and Reactive Phase Formation in Electronic Materials VI: Session IV	Phase Stability, Phase Transformations, and Reactive Phase Formation in Electronic Materials VI: Session V		Oceanic 2

ROOM	Monday		Tuesday		Wednesday		Thursday
	AM	PM	AM	PM	AM	PM	AM
Oceanic 3	2007 Nanomaterials: Fabrication, Properties and Applications: Session I	2007 Nanomaterials: Fabrication, Properties and Applications: Session II	2007 Nanomaterials: Fabrication, Properties and Applications: Session III	2007 Nanomaterials: Fabrication, Properties and Applications: Session IV	2007 Nanomaterials: Fabrication, Properties and Applications: Session V	2007 Nanomaterials: Fabrication, Properties and Applications: Session VI	
Oceanic 4	Wide Band-Gap Semiconductor Nanostructures: Session I	Wide Band-Gap Semiconductor Nanostructures: Session II	Wide Band-Gap Semiconductor Nanostructures: Session III	Wide Band-Gap Semiconductor Nanostructures: Session IV	Integrated Computational Materials Engineering: Lessons from Many Fields: ICME in Materials Science - and - NSF Workshop: CyberInfrastructure to CyberDiscovery for Materials Science	Integrated Computational Materials Engineering: Lessons from Many Fields: ICME in Other Fields - and - National Academies ICME Study Community Town Hall Meeting	General Abstracts: EMPMD: ZnO Thin Films and Liquid Crystals
Oceanic 5	Towards Functional Nanomaterials: Synthesis, Characterization, and Applications: Directed Nano Fabrication	Towards Functional Nanomaterials: Synthesis, Characterization, and Applications: Nano Magnetism, Ferroelectric, Mechanics, and Other Properties	Towards Functional Nanomaterials: Synthesis, Characterization, and Applications: Nanoscale Superstuctures, Metallic Nanoparticles and Plasmon	Towards Functional Nanomaterials: Synthesis, Characterization, and Applications: Nanowires and Nanotubes	Towards Functional Nanomaterials: Synthesis, Characterization, and Applications: Quantum Dots	Innovations in Electrometallurgy: Session I	Innovations in Electrometallurgy: Session II
Oceanic 6	Recent Developments in Semiconductor, Electro Optic and Radio Frequency Materials: Recent Advances in Semiconductor Technologies	Recent Developments in Semiconductor, Electro Optic and Radio Frequency Materials: Progress in Semiconductor Optoelectronics and Beyond	Metrologies for Advanced Materials and Devices: Characterization, Measurement and Testing Science: Metrology for Micro and Nano Structures	Materials in Clean Power Systems II: Fuel Cells, Solar, and Hydrogen-Based Technologies: Hydrogen Storage Materials in Conjuction with the 8th Global Innovations Symposium: Metal Powders for Energy Production and Storage Applications	8th Global Innovations Symposium: Metal Powders for Energy Production and Storage Applications: Session I in Conjuction with the Symposium on Materials for Clean Power Systems II - Hydrogen Storage	8th Global Innovations Symposium: Metal Powders for Energy Production and Storage Applications: Session II	
Oceanic 7	General Abstracts: EMPMD: GaN and Interconnects	Hume-Rothery Symposium: Scattering Studies and the Fundamental Properties of Materials: Session I	Hume-Rothery Symposium: Scattering Studies and the Fundamental Properties of Materials: Session II	Hume-Rothery Symposium: Scattering Studies and the Fundamental Properties of Materials: Session III	Hume-Rothery Symposium: Scattering Studies and the Fundamental Properties of Materials: Session IV	Hume-Rothery Symposium: Scattering Studies and the Fundamental Properties of Materials: Session V	General Abstracts: EMPMD: Magnetic and Ferroelectric Materials
Oceanic 8	Characterization of Minerals, Metals, and Materials: Characterization of Structure across Length Scales I	Characterization of Minerals, Metals, and Materials: Characterization of Structure across Length Scales II	Characterization of Minerals, Metals, and Materials: Characterization of Mechanical and Physical Properties of Materials I	Characterization of Minerals, Metals, and Materials: Characterization of Mechanical and Physical Properties of Materials II	Characterization of Minerals, Metals, and Materials: Characterization of Processing and Properties of Materials	Characterization of Minerals, Metals, and Materials: Characterization of Processing of Materials I	Characterization of Minerals, Metals, and Materials: Characterization of Processing of Materials II

Monday		Tuesday		Wednesday		Thursday	ROOM
AM	PM	AM	PM	AM	PM	AM	
Outreach Programs in Materials Science and Engineering: Outreach Programs at Universities	Outreach Programs in Materials Science and Engineering: Outreach Programs in Industry and Government Laboratories						Pacific Hall A
General Abstracts: LMD: Session I	General Abstracts: LMD: Session II			EMPMD Symposium: Advanced Metallizations and Interconnect Technologies, in Honor of Prof. K. N. Tu's 70th Birthday: Advanced Metallizations and Interconnect Technology I	EMPMD Symposium: Advanced Metallizations and Interconnect Technologies, in Honor of Prof. K. N. Tu's 70th Birthday: Advanced Metallizations and Interconnect Technology II		Pacific Hall B
The Material Recycling Industry: Global Challenges and Opportunities: Plenary Session	General Abstracts: EPD: Hydrometallurgy, Metal Recovery	General Abstracts: EPD: High Temperature Processing	Aluminum Reduction Technology: Modelling and Design I	Aluminum Reduction Technology: Modelling II and General		Electrode Technology Symposium (formerly Carbon): Rodding and Coke Inventory	Southern 1
Aluminum Reduction Technology: Environmental and Plant Improvements	Aluminum Reduction Technology: Operational and Technology Improvements	Aluminum Reduction Technology: Slotted Anodes - Joint Session with Electrode Technology Symposium (formerly Carbon)	Aluminum Reduction Technology: Cell Fundamentals, Phenomena and Alternatives	Aluminum Reduction Technology: Anode Effects and Process Control I	Aluminum Reduction Technology: Inert Anode Operation and Low Temperature Electrolyte	Aluminum Reduction Technology: Process Control II and Bath Chemistry	Southern 2
Electrode Technology Symposium (formerly Carbon): Cathode Part I: Cathode Wear and Construction	Electrode Technology Symposium (formerly Carbon): Anode Technology and Production		Electrode Technology Symposium (formerly Carbon): Properties of Inert Anode Materials	Electrode Technology Symposium (formerly Carbon): Anode Baking Furnace Technology	Electrode Technology Symposium (formerly Carbon): Cathode Part II: Preheating and Cell Start Up	Electrode Technology Symposium (formerly Carbon): Cathode Part III: Titanium Diboride	Southern 3
Magnesium Technology 2007: Magnesium Globalization	Magnesium Technology 2007: Wrought Alloys and Forming Processes I: Deformation	Magnesium Technology 2007: Wrought Alloys and Forming Processes II: Rolling and Forming	Magnesium Technology 2007: Wrought Alloys and Forming Processes III: Extrusions	Magnesium Technology 2007: Alloy Development I	Magnesium Technology 2007: Alloy Development II	Magnesium Technology 2007: Corrosion and Coatings	Southern 4
	Magnesium Technology 2007: Automotive Applications and USAMP Programs	Magnesium Technology 2007: Casting and Solidification I	Magnesium Technology 2007: Casting and Solidification II	Magnesium Technology 2007: Primary Production, Recycling and Environmental/ Welding	Magnesium Technology 2007: Thermal Dynamics and Fundamental Research	Magnesium Technology 2007: Microstructure and Properties	Southern 5

Advances in Computational Materials Science and Engineering Methods: Dedicated Computational Methods

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS: Biomaterials Committee, TMS/ASM: Computational Materials Science & Engineering
Program Organizers: Koen Janssens, Paul Scherrer Institute; Veena Tikare, Sandia National Laboratories; Richard LeSar, Iowa State University

Thursday AM Room: Europe 7
March 1, 2007 Location: Dolphin Hotel

Session Chair: Corbett Battaile, Sandia National Laboratories

9:00 AM Introductory Comments

9:05 AM Invited
Theoretical and Computational Methods for Phase Coarsening: *Ke-Gang Wang*[1]; [1]Florida Institute of Technology

There are some theoretical and computational methods developed for the studies of phase coarsening for the past 50 years. However, there is scant attention to compare the difference, similarity, and unifying property hidden in various theories and simulations. In this paper, I will review Lifshitz, Slyozov, and Wagner' (LSW) theory, and diffusion screening theory, and PrecipiCalc^TM method, multiparticle diffusion simulation, and phase-field simulation. Unified model equations are discovered for phase coarsening. The governing equations in LSW theory, and diffusion screening theory can be derived from the unified model equations with some approximations. The governing equations in multiparticle diffusion simulation and phase field simulation in phase coarsening can also be derived from the unified model equations. The advantages and limitations for different theoretical and computational methods of phase coarsening are compared in details, which can guide scientists and engineers to select computational tools for their needs in microstructure evolution.

9:40 AM Question and Answer Period

9:45 AM
Modeling of Phase Volume Fraction in Alpha + Beta Titanium Alloys by Neural Networks and Genetic Algorithms: *N. Reddy*[1]; Young Hwan Cha[1]; Chong Soo Lee[1]; [1]Pohang University of Science and Technology

A hybrid model of neural networks and genetic algorithms was developed for the analysis and prediction of the correlation between the composition, process parameters, and phase volume fraction in alpha + beta titanium alloys. The inputs of the model consist of alloy composition and quenching temperature and the outputs are phase volume fraction of alpaha and beta phases. Sensitivity analysis on trained neural network model provides a visual selection for choosing inputs for the desired outputs. A Genetic algorithm, biologically inspired soft computing approach was applied to optimize the inputs for the desired outputs. The model predictions are well in agreement with the experimental results. The model would thus reduce the actual number of shop floor trials required to develop Ti alloys of required properties. This would save an enormous amount of time, materials, and cost for industries in designing titanium alloys for the required properties.

10:10 AM Question and Answer Period

10:15 AM
On the Use of Image Moment Invariants to Identify Particle Shapes in Microstructures: *Marc DeGraef*[1]; Jeff Simmons[2]; [1]Carnegie Mellon University; [2]US Air Force

The microstructure of modern engineering materials can be quite complex, consisting of multiple phases and precipitate types. Lifetime extension is a major component of materials development efforts. Since lifetime is often limited by unusual local events that act as defect initiators, the ability to classify qualitative changes in particle morphologies becomes important. It is well known that the moments of an object can be combined to result in parameters that are invariant with respect to rotations, translations, and scaling. Such parameters are known as "moment invariants." We will show that moment invariants can be used as a tool to automate the recognition of object shapes. Furthermore, by combining the moment invariants of second and third order with the Minkowski functionals, one can obtain a detailed description of object shapes. We will illustrate the use of the moment invariants for real super-alloy microstructures and for microstructures generated by phase field methods.

10:40 AM Question and Answer Period

10:45 AM Break

11:15 AM
Free-End Nudged Elastic Band Method to Study Thermally Activated Nanomechanical Processes: Ju Li[1]; *Peter Gordon*[2]; Ting Zhu[3]; [1]Ohio State University; [2]ExxonMobil Research and Engineering; [3]Georgia Institute of Technology

We discuss implementations of the reaction rate theory in solid mechanics, where the reaction coordinate is often the atomic-level inelastic strain distribution. The thermally activated processes we investigate tend to have larger activation volume (i.e. more collective) than chemical reactions and diffusion. Examples of dislocation emission from crack tip [Phys. Rev. Lett. 93, 025503], brittle crack extension [Phys. Rev. Lett. 93, 205504], and chemo-mechanically coupled water corrosion of silica [J. Mech. Phys. Sol. 53, 1597] are used to illustrate the unique features of these problems. The original nudged elastic band method has been modified to study these problems with greater computational efficiency.

11:40 AM Question and Answer Period

11:45 AM
Multiscale Approach to Defects in Carbon Nanotubes and Graphene: *Elif Ertekin*[1]; Murray Daw[2]; Daryl Chrzan[1]; [1]University of California, Berkeley; [2]Clemson University

Stone-Wales defects are expected to play a large role in the mechanical and electronic properties of carbon nanotubes and other graphene systems. These defects are analogs to dislocation dipoles in conventional bulk materials: they may form, dissociate, and travel through the nanotube in response to externally applied loads. To study this unique form of nanoscale plasticity, we develop a multiscale approach to predicting the formation energies of these defects in a variety of geometries. Our approach utilises a continuum, topological description of the defect formation energy which naturally accounts for defect geometry, boundary conditions, and defect-defect interactions. Comparison with results obtained from rigorous total energy electronic structure methods illustrates that our approach can effectively predict formation energies without recourse to expensive quantum mechanical tools, thus facilitating investigations of novel phenomena in carbon nanotubes such as strain-hardening via dislocation dynamics simulations or brittle-ductile transitions via stochastic modeling.

12:10 PM Question and Answer Period

Aluminum Alloys for Transportation, Packaging, Aerospace and Other Applications: Alloys Mechanical Behavior

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee
Program Organizer: Subodh Das, University of Kentucky

Thursday AM Room: Northern A4
March 1, 2007 Location: Dolphin Hotel

Session Chairs: Subodh Das, University of Kentucky; Marwan Khraisheh, University of Kentucky

9:00 AM
Forming Limits of Friction Stir Welded 5182-6111 TWBs during Biaxial Stretching: *Richard Davies*[1]; Frode Stavehaug[2]; Elizabeth Stephens[1]; Glenn Grant[1]; [1]Pacific Northwest National Laboratory; [2]Battelle

The motivation to reduce both weight and cost of automobiles has resulted in broad deployment of tailor welded blanks (TWBs). Conventional, low-

strength steels are predominant in applications. However, the desire to further reduce weight is currently driving the deployment of aluminum. Aluminum alloys are difficult to fusion weld due to the local strength degradation in the weld region and the heat-affected zone (HAZ). This has led to considerable development efforts in aluminum friction stir welding (FSW). This work investigates TWBs comprised of AA5182 joined to AA6111 via FSW, and focuses on characterizing their mechanical properties in and around the weld, as well as their limits of formability under biaxial stretching. The work includes real-time characterization of these TWBs during biaxial stretching using optical strain measurement methods, statistically summarizes the observed limits of TWB formability, and generates forming limit diagrams for the TWBs using an M-K method approach.

9:25 AM

Determining Aluminum Alloy Strain Localization under Biaxial Loading Using In-Situ Optical Strain Imaging: *Elizabeth Stephens*[1]; Frode Stavehaug[2]; Richard Davies[1]; Glenn Grant[1]; [1]Pacific Northwest National Laboratory; [2]Battelle

Strain grid analysis is commonly used to quantify plastic strain accumulation during sheet metal forming. However, the resolution is limited by the grid size and the local strain evolution history cannot be captured. Speckle Pattern Interferometry, on the other hand, has very high resolution and has the ability to capture the local, heterogeneous strain history. This work presents a comparison of results obtained by strain grid analysis and by Speckle Pattern Interferometry on aluminum alloys. In addition, in-situ optical strain imaging utilizing Speckle Pattern Interferometry was used to investigate the strain localization of various aluminum alloys under both uniaxial and biaxial loading conditions. The evolution of strain localization from the early onset of strain localization to final fracture will be presented. Finally, a detailed description of the evolution of strains and strain-rates under both uniaxial and biaxial loading conditions will be presented.

9:50 AM

Characterization of the Evolution of the Properties of Aluminium Alloys: *Christophe Thiebaut*[1]; Laurence Durut[1]; Thierry Vauzelle[1]; Jean François Mariage[1]; Serge Contreras[1]; [1]Commissariat a L'Energie Atomique

Aluminium alloys are now widely used in quite every major applications: automobile, aircraft, consumer goods, … They have a lot of advantages: they are light, have good mechanical properties, are easily forged and machined and some are compatible with hydrogen use. So we have begun studies of the use of aluminium alloys for hydrogen storage under pressure, more precisely with Al-Zn-Mg alloys. These are easily weldable.Most of the results that are in the literature consist in MIG welds. After forming and welding by electron beam technique, we make a heat treatment. Experiments are then made in order to compare the resistance to breakdown of the storage container by hydraulic test. This can be done at different aging of the containers. It can then be compared with the characterization of the containers in terms of hardness and metallurgical characterization (grain size, precipitates, concentration measured by EPMA).

10:15 AM

Solution and Aging Heat Treatment of a Cast Al-Si Alloy: *Sergio Haro Rodriguez*[1]; Julián Ramírez[1]; Simitrio I. Maldonado[1]; Enrique Martinez[2]; Dheerendra Dwivedi[3]; [1]Universidad Autónoma de Zacatecas; [2]Instituto Tecnológico de Zacatecas; [3]Indian Institute of Technology

In the present paper the influence of solutionizing (504-545°C) and aging (154-200°C) temperatures on microstructure and mechanical properties of the A 319 (Al-6.5Si-0.86Fe-2.3Cu) cast aluminum alloy has been reported. The effect of these heat treatment parameters has been investigated with reference to microstructure and mechanical properties. Scanning electron microscopy (SEM) of tensile fractured surfaces was carried out to investigate the influence of solutionizing and aging temperatures on the mode of fracture. Finally, the heat treatment parameters to obtain the better mechanical properties are presented.

10:40 AM Break

10:50 AM

Effect of Aging Treatment on the Mechanical Properties of Thixoextruded 7003 Al Wrought Alloy: *Young-Ok Yoon*[1]; Hoon Cho[1]; Shae K. Kim[1]; Hyung-Ho Jo[1]; [1]Korea Institute of Industrial Technology

The 7003 Al wrought alloy has been used for structural applications where high mechanical strength is needed and in the automotive industry. The 7003 Al wrought alloy obtain full strength after approximately one month storage at room temperature. In the present study, the influences of thixoextrusion parameters, such as isothermal holding temperature of billet, initial ram speed and bearing length, on mechanical properties of thixoextruded 7003 Al wrought alloy were investigated. The results of thixoextrusion experiments about microstructures and mechanical properties were compared with conventional extrusion results. Also, the effect of aging treatment on the mechanical properties of thixoextruded 7003 Al wrought alloy was investigated. The tensile strength and hardness of thixoextruded 7003 Al wrought alloy were increased after aging treatment.

11:15 AM

Research on Electromagnetic Shielding Property of Aluminum Foam: *Haijun Yu*[1]; Guangchun Yao[1]; Yihan Liu[1]; [1]Northeastern University

Al-Si closed-cell aluminum foams of different densities were prepared by using molten body transitional foaming process in Northeastern University of China through adjusting foaming temperature, foaming time, heat preservation time and vesicant addition amount and other technological parameters. Testing its electromagnetic shielding effectiveness using method of falan coaxial, the results show that the shielding effectiveness of material is affected obviously by the frequency of electromagnetic interference. With the interference frequency increasing from 10 MHz to 600MHz, shielding effectiveness of aluminum foam decreases gradually; and increases when frequency is added from 600 MHz to 1500 MHz. The influence of relative density on electromagnetic shielding effectiveness is not obvious.

11:40 AM

The Effect of Equal Channel Angular Pressing (ECAP) on the Fracture Toughness of High Solute Aluminum Alloys: *Christopher Hovanec*[1]; Roger Doherty[1]; Surya Kalidindi[1]; [1]Drexel University

In the present investigation aluminum alloys with varying amounts of solute have been subjected to large strains by equal channel angular pressing (ECAP). This novel process is capable of imposing very large plastic strains (>10) without major changes in billet dimensions. The ensuing submicron-grain structures result in large yield strengths, as predicted by solute enhanced strain hardening and increased by Hall-Petch grain size strengthening. In addition, grain-boundary precipitates formed during traditional age-hardening treatments, which are known to degrade fracture toughness, are avoided. The yield strength and fracture toughness after strain hardening were determined and then compared to those produced by traditional precipitation methods. The analysis is expected to confirm that aluminum alloys processed by strain hardening (cold rolling and ECAP) exhibit substantial improvements fracture toughness at comparable yield strengths.

12:05 PM

The Effects of Mn Additions on the Microstructure and Mechanical Properties of Type 319 Aluminum Alloys: *Junyeon Hwang*[1]; Herbert Doty[2]; Michael Kaufman[1]; [1]University of North Texas; [2]GM Powertrain Group, Metal Casting Technology Inc.

The microstructure and mechanical properties of Type 319 aluminum casting alloys have been examined as a function of Mn content. As the Mn content is increased up to ~0.4 wt. pct., corresponding to a Fe/Mn ratio of ~1.3 in the baseline alloy (Al-7wt%Si-3.8wt%Cu-0.5wt%Fe), the detrimental plate-like β-Al_5FeSi intermetallic phase is modified to the less-detrimental, Chinese script α-$Al_{12}[Fe, Mn]_3Si_2$ phase resulting in improved tensile properties. However, greater amounts of Mn are observed to reduce the mechanical properties by increasing the total amount of these undesirable intermetallic phases. The mechanical properties are correlated with both microstructural observations and fractography results in order to draw conclusions concerning the role of Mn in enhancing the properties of these important commercial alloys. [Research supported by GM Powertrain. Characterization work performed using the analytical facilities in the Center for Advanced Research and Technology at the University of North Texas].

Aluminum Reduction Technology: Process Control II and Bath Chemistry

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee
Program Organizers: Geoffrey Bearne, Rio Tinto Aluminium Ltd; Stephen Lindsay, Alcoa Inc; Morten Sorlie, Elkem Aluminium ANS

Thursday AM Room: Southern 2
March 1, 2007 Location: Dolphin Hotel

Session Chair: Oliver Martin, Alcan Inc

9:00 AM
Bath Superheat to Control Electrolysis Process: *A. Berezin*[1]; Tatiana Piskazhova[1]; V. Gritsko[2]; A. Tarakanov[2]; I. Volokhov[3]; P. Polyakov[4]; [1]Engineering and Technology Center, Ltd.; [2]Mayak PKF Ltd.; [3]Engineering and Technology Center Ltd.; [4]State University of Non-Ferrous Metals and Gold

The paper presents a control system developed by the authors on the basis of bath superheat measurements. To measure the superheat a special in-house device has been developed. Software automatically transmitting control actions to the aluminum electrolysis computer process control system has been developed for commercial implementation. The program calculated aluminum fluoride and cell voltage additions to bring the liquidus and superheat temperature to their target. The calculation algorithms to correct additions have been produced by bath and liquidus temperature measurements made under different process situations and mathematical modeling and expert analysis by process engineers. To logically combine miscellaneous information the program was built on fuzzy logics principles.

9:25 AM
Aluminum Reduction Cell Control by Distributed Temperature Data: *Vladimir Yurkov*[1]; [1]RUSAL

Bath temperature is among the key process variables in aluminum reduction. A system to continuously and automatically control the bath temperature would be ideal. In practice the bath temperature is measured manually once a day or once in several days. These measurements are recorded in the process database. However, to use these discrete data directly to continuously control the thermal conditions of electrolysis is difficult. The author has developed anexperimental system to continuously evaluate bath temperature by distributed temperature data, based on a mathematical model of the reduction process. Occasional manual bath temperature measurements and continuous information from thermocouples in the cathode are used. Signals from this virtual bath temperature sensor are transmitted to the thermal conditions control system.

9:50 AM
Use of Contigency Tables for Determining Statistical Dependence of Attribute Data from Aluminum Reduction Cell Processes: *Kayron Lalonde*[1]; Wayne Cotten[1]; [1]Alcoa Inc

A statistical method called Contingency Tables was used to determine if a high cell failure rate in an aluminum production line was related to the accumulation of insulating material along the cell side and collector bar electrical joints. Contingency Table analysis of attribute data showed the cell failures and insulating material were statistically related at a 99% confidence level. Therefore, removal of the material and repair of broken electrical joints were critical to reducing cell failures in this production line.

10:15 AM
Adaptive Fuzzy Control System of 300kA Aluminum Production Cell: *Zeng Shuiping*[1]; Li Jinhong[1]; [1]North China University of Technology

An adaptive fuzzy logic control system has been designed for a 300kAprebake aluminum production cell. It includes the prediction and adjustment of some parameters. The system controls the bath temperature, bath liquidus temperature and anode effect frequency by adjusting the AlF3 additions, aluminum tapping magnitude, cell voltage setpoint and the alumina feeding interval. In addition to the cell voltage, bath mperature and bath ratio, the inputs of the system include the bath superheat and cathode voltage drop, measured by use of the Heraeus equipment. The control system have been running for six months in the Yichun aluminum plant in Hennan province of China. Current efficiency of up to 95%, anode effect frequency down to 0.15 anode effects/cell/day and energy consumption of 13.2DCkWh/kg have been achieved.

10:40 AM Break

10:55 AM
Predictive Models for the Density and Viscosity of the NaF-AlF_3-CaF_2-Al_2O_3 Electrolyte: *Christian Robelin*[1]; Patrice Chartrand[1]; [1]CRCT (Ecole Polytechnique de Montreal)

A thermodynamic database was previously developed for the NaF-AlF_3-CaF_2-Al_2O_3 system involved in the alumina reduction cells. The liquid model was the Quasichemical Model in the Quadruplet Approximation evaluating 1st- and 2nd-nearest-neighbor short-range order. Density and viscosity models were developed recently. The density is easily derived from the molar volume, defined as the pressure derivative of the molar Gibbs energy at fixed temperature and composition. Therefore, by introducing in the Gibbs energy of the phase temperature-dependent molar volume expressions for the pure components and pressure-dependent excess parameters for the binary subsystems, it was possible to reproduce, and eventually predict, the density of the multicomponent liquid. The viscosity was modeled using an Eyring equation with a viscous activation energy expanded as a 1st-order polynomial in the quadruplet mole fractions (calculated from the thermodynamic model). The model parameters form databases for use with the FactSage thermochemical software.

11:20 AM
Modified Alumina-Cryolite Bath with High Electrical Conductivity and Dissolution Rate of Alumina: *Anton Frolov*[1]; Alexander Gusev[1]; Yurii Zaikov[2]; Andrey Khramov[2]; Nikolai Shurov[2]; Olga Tkacheva[2]; Alexei Apisarov[2]; Vadim Kovrov[2]; [1]Engineering-Technological Center Ltd, RUSAL; [2]Institute of High Temperature Electrochemistry

To improve the commercial electrolysis of aluminum at high current density a modified bath with better electrical conductivity and better dissolution rate of alumina has been developed. The bath modified has been developed on the basis of sodium cryolite Na3AlF6 with additions AlF3, KF, LiF, CaF2, MgF2. Physical-chemical properties: electrical conductivity, solubility and dissolution rate of alumina, liquidus temperature have been measured experimentally. Electrical conductivity of the modified bath has been found to be 15-20% higher than electrical conductivity of commercial alumina-cryolite bath. And dissolution rate of alumina of the modified bath has been found to be 3X higher than dissolution rate of commercial alumina-cryolite baths. Effect of KF concentration, alumina content and temperature on these properties have been studied experimentally. The modified bath developed has been tested on an industrial cell with prebaked anodes; during the test the cell voltage was decreased by 0.2 V with anode-cathode distance unchanged.

11:45 AM
Graphitised Cathode Flaking Phenomenon during Alba's Line-5 Start-Up: *Mohamed Mahmood*[1]; [1]Bahrain Aluminium Company (ALBA)

In year 2005 Aluminium Bahrain Alba increased the metal production capacity to 840,000 mt/year with the start up of the new potline-5, which is equipped with 336 pots operating at 336 KA. At the rate of 4 pots per day, Pot line-5 is started in a worldwide record breaking of 77 days. During the first days of start up, the team faced a big challenge when suddenly all the started pots behaved very abnormal due to floating of carbon pieces in the bath. These carbon pieces found to be flakes from cathodes blocks. To control the pots, the floating carbon pieces were fished out by continues manual skimming. A detailed study on this Phenomenon revealed the main cause being high concentration of localised sodium salt combined with higher operating pot voltage causing higher gradient of thermal expansion with in the cathode blocks and hence resulting into flaking of top surface of cathode into pieces of carbon.

12:10 PM
Fault Diagnosis System for 350kA Pre-Baked Aluminum Reduction Cell Based on BP Neural Network: *Zeng Shuiping*[1]; [1]North China University of Technology

The spectrum of the cell resistance shows the main frequency domain is 0~0.1Hz and there is an obvious wave crest in higher frequency. Considering

the three different states of the aluminum reduction cell, which are normal production, fluctuation of fluid aluminum and abnormal state of anode, the paper collects the many fault samples, takes the frequency and spectrum energy as eigenvectors, and sets up a three-layer BP neural network model, which is input-layer, middle layer and output-layer. Input-layer contains ten nerve cells and output-layer contains three nerve cells. The model is tested by using the practical data from 350kA pre-baked aluminum reduction cells. The results indicate that the system can diagnose the faults in the precision of 80%.

Biological Materials Science: Biological Materials II

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee
Program Organizers: Andrea Hodge, Lawrence Livermore National Laboratory; Chwee Lim, National University of Singapore; Eduard Artz, University of Stuttgart; Masaaki Sato, Tohoku University; Marc Meyers, University of California, San Diego

Thursday AM Room: Europe 4
March 1, 2007 Location: Dolphin Hotel

Session Chair: Andrea Hodge, Lawrence Livermore National Laboratory

9:00 AM
Enhancement of Biocompatibility on Bioactive Ti-Nb-Based Alloy by High-Density Plasma Modification: *En-Yu Wu*[1]; Keng-Liang Ou[2]; Yung-Ning Pan[1]; Chang-Chih Chen[3]; [1]National Taiwan University; [2]Taipei Medical University; [3]Mackay Memorial Hospital

X-ray photoelectron spectroscopy, grazing incident X-ray diffraction, transmission electron microscopy and scanning electron microscopy as well as cell culture were conducted to evaluate the oxidation effect on the formation of nanoprecipitates on Ti-Nb-Fe-Hf alloy during plasma modification. Nanoprecipitates (metal oxides) was formed after plasma oxidation, and served as a crosslinking acceptor during plasma polymerization to enhance the tissue healing. Plasma oxidation occurred and multi-nanoprecipitates were formed by high-density plasma modification. The nanoprecipitates play an important role in enhancing the biocompatibility. The formation of nanoprecipitates by oxidation treatment and of the functional groups linking on nanoprecipitates by polymerization is believed to improve biocompatibility, thereby promoting osseointegration.

9:20 AM
Nucleation and Growth of Needle-Like Fluorapatite Crystals: *Yong Liu*[1]; Xiaoxian Sheng[1]; Qijun Xiang[1]; Xiaohong Dan[1]; [1]State Key Laboratory of Powder Metallurgy, Central South University

The nucleation behaviors of glass-ceramics with different mica/apatite ratios were investigated. By using DTA, SEM and XRD, the effect of CaO and P2O5 addition on the nucleation behaviors at 650° for 1h was studied. Results showed that the addition of CaO and P2O5 promotes nucleation process and leads to the formation of different nucleation phases. The nucleation occurred in the order of MgF2, CaF2 and Ca5(PO4)3F crystals with the addition of CaO and P2O5 increasing. Further, Ca5(PO4)3F nucleus was observed to grow along the c axis, which resulted in the growth of needle-like apatite by controlling the heat treatment process.in this glass-ceramic biomaterial. The formation of needle-like fluorapatite crystals, instead of particle-like crystals reported in previous studies, can be attributed to the one-dimensionally rapid growth of fluorapatite along the c-axis. Since needle-like fluorapatite crystals are of the same morphology in human bones, they show excellent bioactivity in vivo.

9:40 AM
Surface Structure Modification and Recrystallization of Pulsed Laser Deposited Amorphous Calcium Phosphate Films: *Saulius Drukteinis*[1]; Renato Camata[1]; Hyunbin Kim[1]; [1]University of Alabama at Birmingham

Calcium phosphate films produced below 400°C using pulsed laser deposition (PLD) are amorphous. We developed a method utilizing the high dissolution rate of this material in aqueous medium and its propensity to crystallize under heat treatments, to create novel calcium phosphate coatings with a wide range of crystalline surface micro-morphologies. Hydroxyapatite targets were ablated using a KrF excimer laser at various energy densities and Ar/H2O pressures. Silicon samples sputtered with titanium were used as substrates. Following PLD of amorphous calcium phosphates, controlled dissolution patterns were created with substrate cooling under a constant Ar:H2O flow with variable H2O concentrations. This was followed by heat treatment of the samples, between 300°C and 600°C. X-ray diffraction and optical microscopy revealed the formation of calcium phosphate crystalline phases in the samples with various surface micro-morphologies for heat treatments at temperatures as low as 400°C. In-vitro fibroblast response to these films was analyzed with SEM.

10:00 AM
Structural Evolution via Elastocapillarity-Driven Coalescence of Filaments: *Ramanathan Krishnamurthy*[1]; David Srolovitz[1]; [1]Princeton University

A competition between elasticity and capillarity results in the generation of complex patterns during the self-assembly of flexible filamentary structures. Such clustering/coalescence commonly occurs in many physically and biologically interesting phenomena, including the bundling of hairs in the tarsi of insects, in biomimetic adhesives and in the sintering of topcoat columns in thermal barrier coatings. We present a novel modeling approach to study the structures generated from such coalescence processes. The coalescence of filament pairs is modeled via a variational approach that includes dissipation (typically diffusional) and a free energy with elastic and surface energy contributions. This approach is incorporated into a simulation of the dynamics of large numbers of discrete filaments to predict the evolution of cluster patterns. Cluster distributions depend intimately on filament aspect ratio, density, elastic moduli and adhesion strength. The resulting patterns and cluster size distributions will be compared with scaling results from experiments.

10:20 AM
Improving Wear Resistance of UHMWPE by Mechanical Processing: *Dongsheng Li*[1]; Hamid Garmestani[1]; [1]Georgia Institute of Technology

Wear resistance of conventional UHMWPE samples with different microstructure is studied. Investigation on the relationship between wear resistance and microstructure UHMWPE shows that the molecular orientation distribution plays a critical role in wear resistance. The anisotropy of wear properties is related directly to crystal orientation distribution. We studied microstructure and properties evolution during different mechanical deformation path to establish a preliminary database on process, microstructure and properties. This will enable further process design to improve wear resistance.

10:40 AM Break

10:50 AM
Micro Particles Formation, Characterization and Application of Biodegradable Polyurethane for Controlled Released of Theophilline: *Morteza Mahmoudi*[1]; [1]Amirkabir University of Technology

Polyurethane microspheres having diameter in the range of 30-280 µm were prepared by condensation polymerization. Microencapsulation of theophylline in polyurethane was developed with Hexamethylen diisocyanat (HMDI), Polycaprolactone (PCL) and Botane diol (BD) as chain extender. Polyurethane microspheres were prepared in two reactors for pre-polymer preparation and microspheres formation. PCL, HMDI and theopylline were mixed in the first reactor before suspending the mixture in aqueous medium (moving at 5000 rpm) of the second reactor. Samples were divided in four groups, A, B, C and D groups. These microspheres were characterized by various techniques such as scanning electron microscopy (SEM), optical microscopy and particle size analyzer. Particle size investigation with optical microscopy and particle size analyzer(by pro plus software) revealed size distribution of 30-280 µm. Also it was found that B group had a smaller size than A group because of presence of starch. Scanning electron microscopy (SEM) was used to study morphology of samples. SEM illustrated many microspheres with spherical morphology.

11:10 AM

The Influence of Chloride Ion to the Biooxidation of Arsenic Bearing Gold Concentration: *Dawen Wang*[1]; Hongying Yang[1]; Changliang Zhu[1]; Huanjie Jiang[1]; [1]Northeastern University

During the process of arsenic bearing gold concentration biooxidation, the content of chloride ion in water is a very important factor to the activity of bacteria and the oxidation of sulfide minerals. In this paper, the influence of underground mine water with different chloride ion content to the biooxidation of arsenic bearing gold concentration and the limit of chloride ion content to bacteria were summarized. These results indicated if the content of chloride ion was less than 1.2g/L, the bacteria's ability to oxidize sulfide minerals was little affected, and if the content of chloride ion were increased to 2g/L or more, the activity of bacteria was seriously restrained, and if the content of chloride ion were increased to 4g/L, the activity of bacteria was absolutely restrained.

11:30 AM

Use of Waste Biomaterials for Removal of Heavy Metals from Effluents: *Sarabjeet Ahluwalia*[1]; Dinesh Goyal[1]; [1]Thapar Institute of Enginnering and Technology

Intensive industrialization has generated huge amount of toxic heavy metals into the environment and problem of coping with the presence of heavy metals has become one of the top priorities in water and wastewater treatment. Conventional treatment technologies are inadequate to remove heavy metal contamination. Biomaterials derived from bio-waste such as waste tea leaves, paper mill sludge and microbial wastes from distillery and pharmaceutical industry were investigated for removal of heavy metals from aqueous solutions in batch and continuous flow sorption columns. A flow through biosorption column packed with paper mill sludge, distillery waste, waste tea-leaves and bio-waste attained a sorption capacity of 238, 4.54, 74 and 33 mg Pb g-1 of biomass respectively, whereas bio-waste also showed sorption capacity of 12.6 mg Cr(VI) g-1.Such biomaterials are available in large quantity and can find application as an alternative to existing commercial adsorbents for removal of metals from wastewater.

Bulk Metallic Glasses IV: Processing and Mechanical Properties IV

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

Program Organizers: Peter Liaw, Univ of Tennessee; Raymond Buchanan, University of Tennessee; Wenhui Jiang, University of Tennessee; Guojiang Fan, University of Tennessee; Hahn Choo, University of Tennessee; Yanfei Gao, University of Tennessee

Thursday AM
March 1, 2007

Room: Asia 1
Location: Dolphin Hotel

Session Chairs: Y. F. Gao, University of Tennessee; K. M. Flores, Ohio State University

9:00 AM Invited

Processing Opportunities of Bulk Metallic Glass: *Jan Schroers*[1]; [1]Yale University

In contrast to most crystalline metallic materials, bulk metallic glasses (BMG) do not require post-cast processing or heat treatment and all properties are already achieved in the as-cast state. This, together with the absence of a phase transition and the sluggish crystallization kinetics opens up an opportunity for a wide range of processing methods. Fundamentally, they can be separated into two categories. BMG can be directly cast. Critical cooling rates for a wide range of BMGs are lower than 100 K/s. This however can still be challenging for the casting process since during casting cooling and filling of the entire mold cavity has to occur simultaneously. This limits the complexity of the geometries that can be produced by this method even when processing parameters are carefully balanced. Alternatively, BMG can be superplastically formed in the supercooled liquid region where the BMG exist as a highly viscous metastable liquid. In this case the required fast cooling and forming are decoupled. The BMG is formed in a high viscous state where it behaves very similar to plastics when compared by processing temperature and forming pressure. A measure to qualify the formability of a BMG will be introduced together with parameters that correlate with the BMG's formability. Potentials and challenges will be discussed and various examples of the use of this processing opportunity will be given.

9:20 AM Invited

Oxidation Behavior of Cu-Based Glassy Alloys at 400-550°C in Dry Air: Hsin-Hsin Hsieh[1]; Tsu-Hsin Ho[1]; Yan-Rong Chen[1]; *Wu Kai*[1]; D. C. Qiao[2]; F. Jiang[2]; Peter Liaw[2]; G. Fan[2]; Hahn Choo[2]; [1]National Taiwan Ocean University; [2]University of Tennessee

The oxidation behavior of the $Cu_{47.5}Zr_{47.5}Al_5$ (Cu3) and $Cu_{47}Ti_{34}Zr_{11}Ni_8$ (Cu4) bulk-metallic glasses (BMGs) was studied over the temperature range of 400 - 550°C in dry air. The oxidation kinetics of both Cu-based BMGs generally followed a multi-stage parabolic-rate law, with their steady-state-rate constants (K_p values) fluctuating with temperature. The scales formed on the two glassy alloys consisted of mostly tetragonal-ZrO_2 (t-ZrO_2), monoclinic-ZrO_2 (m-ZrO_2), Al_2O_3, Cu_2O, and CuO. Furthermore, the amorphous substrate of Cu3 transformed into three crystalline phases of ZrCu, Zr_2Cu, and Cu_2ZrAl after the oxidation at T > 400°C, while $Cu_{51}Zr_{14}$ and CuTi were detected for Cu4 at higher temperatures. It was found that the oxidation mechanism of BMGs is strongly dependent on temperature and alloy composition.

9:40 AM Invited

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

In the present study, we attempt to prepare the amorphous/amorphous composite alloys through powder metallurgy route. The preparation of amorphous/amorphous composite alloy powders was accomplished by the ball milling of the mixture of Ti50Cu28Ni15Sn7 and Ni60Nb20Zr20 glassy powders. The bulk amorphous/amorphous composite alloys was successfully prepared by vacuum hot pressing the as-milled composite powders at the supercooled liquid region of Ti50Cu28Ni15Sn7 glassy powders under a pressure of 1.2 GPa. The mechanical behavior of the bulk amorphous/amorphous composite alloys was investigated by hardness test. The measured hardness values follow the rule-of-mixture equation for describing the hardness of the composite materials. The potentiodynamic polarization study were conducted in 3.5 wt% NaCl, 0.1N NaOH, 0.1N H2SO4 and 0.1N Na2SO4 solutions, respectively. The corrosion resistance at different solutions as indicated by the passive current density and the corrosion rate will be discussed.

10:00 AM

Laser Processing of Zr- and Cu- Based Bulk Metallic Glasses: Hongqing Sun[1]; Katharine Flores[1]; [1]Ohio State University

Laser processing of metallic glasses offers the possibility of creating and repairing coatings and larger scale components with amorphous or uniquely tailored microstructures. The advantages of the localized melting and rapid solidification during laser deposition also present the opportunity to push beyond the dimensional limitation of traditional casting techniques and explore new glass forming compositions. In the present work, Laser Engineered Net Shape (LENS™) processing is used to deposit metallic glass powders on a bulk metallic glass substrate of related composition. The microstructure, composition, and microhardness of the deposited layers and underlying substrate are characterized as functions of the laser power and travel speed. Amorphous melt zones surrounded by partially crystalline heat affected zones (HAZ) are observed for all processing conditions examined. Numerous different crystal morphologies are observed in the HAZ. The microstructure, thickness, and microhardness of both the melt zone and the HAZ strongly depend on the processing parameters.

10:15 AM

Forming of Mg Bulk Metallic Glasses in the Supercooled Liquid Region: Sylvain Puech[1]; *Jean-Jacques Blandin*[1]; Jean-Louis Soubeyroux[2]; [1]Institut National Polytechnique de Grenoble; [2]Centre National de la Recherche Scientifique de Grenoble

Mg-Cu-RE alloys are produced under the form of amorphous cylindrical rods and characterized by X-ray analyses and differential scanning calorimetry. Their capacity to be formed in the supercooled liquid regions

(SLR) is studied. In the SLR, crystallization can occur and affect strongly the forming conditions. In consequence, the thermal stabilities of the glasses are studied, in particular in the case of a Mg-Cu-Gd glass for which the kinetics of crystallisation are quantified and the associated populations of crystallites identified. By appropriate heat treatments, various fractions of crystallites are thus produced and the effects of crystallization of the viscoplastic properties in the SLR region are discussed in relation with mechanical models developed for materials containing rigid inclusions dispersed in a viscous medium, the possible effect of deformation on crystallization kinetics being considered. Finally forming tests in the SLR domain are also performed.

10:30 AM

Effect of Niobium on Glass-Forming Ability of Fe-Based Alloys by Mechanical Alloying: *Satyajeet Sharma*[1]; Raj Vaidyanathan[1]; C. Suryanarayana[1]; [1]University of Central Florida

Amorphization by mechanical alloying has been achieved in a multicomponent Fe-based alloy system of composition Fe42Ni28Zr10B20. Factors known to affect the glass-forming ability (GFA) of alloys by mechanical alloying include, the alloy composition, number of components, atomic size difference, and heat of mixing of constituent elements. Recently it has been observed that addition of an alloying element with positive heat of mixing has increased the GFA during processing of bulk metallic glasses through the solidification route. We have investigated the GFA in terms of the milling time required to produce the alloy in the glassy state. We have shown that addition of Nb to the above Fe-Ni-Zr-B system has significantly improved the GFA of the alloy as indicated by the decreased milling time required for glass formation. It is also seen that the effect on glass formation was best when the Nb content was limited to about 2 at.%.

10:45 AM Invited

Bulk Metallic Glass: A Very Low Damping Material - Possible Applications: *Jean-Marc Pelletier*[1]; Cédric Haon[2]; Denis Camel[2]; Béatrice Drevet[2]; [1]INSA-Lyon; [2]CEA

In crystalline materials, the physical origin of damping phenomena has been identified: movements of point defects, interstitial atoms, dislocations, grains boundaries, antiphase boundaries… Conversely, in amorphous materials the concept of defect is not so clear and consequently the damping behavior may can be very different. Present work addresses on damping experiments performed in bulk metallic glasses: Pd-Cu-Ni-P and Zr-Ti-Cu-Ni-Be alloys. Due to the very low absorbing level a specific device is required. Indeed quality factor as high as 106 is obtained after an appropriated thermal treatment. This result is discussed considering the thermoelastic origin of the absorbing phenomena. Due to this very low absorbing feature and taking advantage of the metallic nature (which allows a possible electromagnetic excitation to induce vibrations) a possible application is described.

11:05 AM Invited

Fabricating Bulk Metallic Glasses by Powder Metallurgy: *Yong Liu*[1]; Zuming Liu[1]; Shiwen He[1]; Baiyun Huang[1]; [1]State Key Laboratory of Powder Metallurgy, Central South University

Powder metallurgical processing has an advantage over casting process in near net shaping metallic and ceramic components of various complex shapes. This is of significant importance for fabricating bulk metallic glasses, the sizes of which are, so far, still highly dependant on their glass forming ability. It is convenient to consolidate amorphous metallic powders into bulk components of a large size, which is beyond the glass forming ability of the same composition. However, impurities induced by handling powders and crystallization during densification are two major problems, and may result in degradation of physical properties. Recent progress in fabricating bulk metallic glasses by powder metallurgy were reviewed, including amorphous powders, consolidation methods and densification mechanisms, mechanical properties and magnetic properties.

11:25 AM

Deciphering Local Atomic Coordination in Multi-Component Bulk Metallic Glasses: Dong Ma[1]; Alexandru Stoica[1]; L. Yang[1]; *Xun-li Wang*[1]; Z. Lu[1]; J. Neuefeind[1]; Matthew Kramer[2]; James Richardson[3]; Th. Proffen[4]; [1]Oak Ridge National Laboratory; [2]Ames Laboratory, Iowa State University; [3]Argonne National Laboratory; [4]Los Alamos National Laboratory

Unlike oxide glasses (e.g., SiO_2) featuring covalent bonds and simple chemical make-ups, bulk metallic glasses are characterized by weaker metallic bonding and complex multiple chemical interactions, making the determination of their amorphous structures a significant challenge. Here we report complimentary use of high energy x-ray and time-of-flight neutron diffraction techniques to probe the local atomic structure in a Zr-based bulk metallic glass by means of the pair distribution function (PDF) analysis of the total scattering data. Our experimentally resolved coordination numbers indicate the presence of multiple types of solute-centered clusters and the lack of solute-solute bonding, arising from strong chemical short-range ordering around solute atoms. Furthermore, our analysis shows near-unity values for the total local packing efficiency, suggesting that the multi-component amorphous structure is facilitated by local atomic efficient packing.

11:40 AM

Room-Temperature Oxidation of Ca-Based Bulk Amorphous Materials: *Bryan Barnard*[1]; Peter Liaw[1]; Raymond Buchanan[1]; Oleg Senkov[2]; Daniel Miracle[3]; [1]University of Tennessee, Knoxville; [2]UES, Inc., Air Force Research Laboratory; [3]Air Force Research Laboratory

Studies of the oxidation behaviors of three Ca-based bulk metallic glasses (BMGs), Ca65Mg15Zn20, Ca50Mg20Cu30, and Ca55Mg18Zn11Cu16, in air at room temperature were conducted. The oxidation behaviors of the BMGs were compared with those of their crystalline counterparts. The amorphous alloys were found to be more oxidation resistant than their crystalline counterparts. The quaternary alloy demonstrated the greatest resistance to oxidation, while the ternary, Zn-containing alloy demonstrated the least favorable oxidation resistance. Scanning-electron-microscopy (SEM) studies revealed a thick (about 8 mm), loose oxide layer on the surface of the Ca65Mg15Zn20 BMG, while thin (less than 1 mm) oxide layers formed on the surfaces of the other two amorphous alloys after holding in air for at least 14 months. The mechanisms of oxidation in these alloys will also be discussed. Acknowledgement: The financial support of the NSF IGERT Program, and the Air Force Office of Scientific Research are appreciated.

11:55 AM

Inverse Role of Zr76.11Ti4.20Cu4.51Ni3.16Be1.49Nb10.53 Bulk Metallic Glass Composite in Supercooled Liquid Region: *Hyun-Joon Jun*[1]; Kwang Seok Lee[1]; Young Won Chang[1]; [1]Pohang University of Science and Technology

The thermal properties of a Zr76.11Ti4.20Cu4.51Ni3.16Be1.49Nb10.5 3 bulk metallic glass (BMG) have been investigated by using a differential scanning calorimeter (DSC). The composition of dendrite phase was then subsequently analyzed by using an EPMA, XRD, and TEM. The glass transition and crystallization onset temperatures were determined as 339.7°C and 375.8°C for this BMG, respectively. The Zr-Ti-Nb dendrite phase was found to have a BCC structure. Mechanical properties have also been examined by conducting a series of uniaxial compression tests at various temperatures within supercooled liquid region under the strain rates between 10-4 /s and 3×10-2 /s. The hardness of matrix and dendrite was then measured separately. The glassy matrix appears to play major role on the elongation, while dendrite phase on the strength of this BMG composite at high temperatures within supercooled liquid region.

12:10 PM

Compression-Compression Fatigue Behavior of Several Zr-Based Bulk-Metallic Glasses: *Dongchun Qiao*[1]; Gongyao Wang[1]; Y. Yokoyama[1]; Peter Liaw[1]; [1]University of Tennessee

The compression-compression fatigue behavior was studied on the Zr50Al30Cu40, Zr50Al10Ni10Cu30, and Zr50Al10Cu37Pd3 bulk-metallic glasses (BMGs) under a load control, employing an electrohydraulic machine, at a frequency of 10 Hz (using a sinusoidal waveform) with an R ratio of 0.1, where R =σmin./σmax. (σin. and σmax. are the applied minimum and maximum stresses, respectively). The obtained results were compared with those of the three-point bend, four-point bend, and tension-tension fatigue tests. The improvement of the compression-compression fatigue life and fatigue-endurance limit indicated the different fatigue-fracture mechanisms, which were investigated by the fracture-surface observations. The possible different factors (the strength, the plasticity, the Poisson's ratio, the microstructure, and the stress state) that affect the fatigue lives and fatigue-endurance limits of these three BMGs were also discussed.

12:25 PM

Structure of Shock Waves and Hugoniot Elastic Limit of a Zirconium-Based Bulk Metallic Glass: *Fuping Yuan*[1]; Vikas Prakash[1]; John Lewandowski[1]; [1]Case Western Reserve University

In the present study, the bulk metallic glass samples (BMG), Zr41.25 Ti13.75Ni10Cu12.5Be22.5, were shock loaded by utilizing Ti-6Al-4V and WC flyer plates to around 7 GPa and 12 GPa, respectively. The particle velocity profiles, measured at the back surface of the target plate by using the VALYNTM VISAR, were analyzed to (a) better understand the structure of shock waves in BMG subjected to uniaxial shock compression and combined shock compression and shear, and (b) obtain the Hugoniot elastic limit (HEL) of the material. At the highest impact velocities, the measured particle velocity versus time profiles show a step-like elastic precursor to the HEL level, a peak at the elastic front, followed by a steeply rising plastic wave and a gradual transition to a final plateau. The HEL was estimated to be 6.15 GPa. Scanning electron microscopy was used to study the inelasticity in the BMG samples following the shock loading.

12:40 PM

Synthesis and Characterization of Metallic Glass/Metallic Glass Composites: *JinKyu Lee*[1]; MinHa Lee[2]; TaekSoo Kim[1]; JungChan Bae[1]; [1]Korea Institute of Industrial Technology; [2]Ames Laboratory, Iowa State University

The mechanical milling process has the potential to extend the possibility of making novel composition and microstructure, which can not be attained conventional casting process. Solid-state amorphization processing can easily form amorphous alloys at compositions difficult to achieve by using conventional rapid cooling process. Recently, bulk metallic glass composites have been prepared successfully by mechanical milling process with subsequent consolidation process. In this study, we report the formation route of metallic glass/metallic glass composites by a controlled milling process with subsequent consolidation process. Cu-based and Zr-based metallic glass powders produced by high pressure gas atomization were used as starting materials. To produce the composites, two different metallic glass powders were mechanical milling, and then consolidated in their supercooled liquid region using a spark plasma sintering method. The structure of the as-milled powders and consolidated materials was characterized by X-ray diffractometry (XRD), Scanning electron microscopy (SEM) and transmission scanning microscopy (TEM).

Cast Shop Technology: Cast Shop Safety

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee
Program Organizers: David DeYoung, Alcoa Inc; Rene Kieft, Corus Group; Morten Sorlie, Elkem Aluminium ANS

Thursday AM Room: Northern E1
March 1, 2007 Location: Dolphin Hotel

Session Chair: Seymour Epstein, Aluminum Association

9:00 AM Introductory Comments

9:05 AM

An Update on the Reported Causes of Molten Metal Explosions: *Seymour Epstein*[1]; [1]Aluminum Association, Inc.

In spite of extensive efforts by the aluminum industry to gain a better understanding of molten aluminum-water explosions and how they can be prevented, explosions continue to occur. A valuable insight into the causes of many of the explosions occurring in recent years has been provided by the world-wide molten metal incident reporting program instituted by The Aluminum Association in 1985. The reports submitted to the Association and shared with the more than 200 program participants serve to enhance awareness, to provide information for employee safety training and to provide guidance for the industry's programs and efforts to prevent these occurrences.

9:30 AM

Scrap Inspection Requires Ingenuity and Management: *Maxwell Bertram*[1]; F. Hubbard[1]; D. Pierce[2]; [1]Aleris International Inc; [2]Consultant

Over the years, secondary aluminum processors have experienced serious molten metal incidents resulting from melting scrap which contained excess water and other contaminants. To better ensure safe melting operations, management must install equipment and develop creative practices to better ensure there are: 1) Means to discover excess water and other contaminants in scrap; 2) Procedures for safe preparation and processing of wet scrap; and, 3) Systems for rejection and reporting for contaminated scrap. Management must further develop systems for communicating expectations and expectations of scrap conditions to suppliers, and contingencies for occasions when scrap supplies do not meet these expectations. Management, at all levels, must be creative in developing better ways to protect people and property from the potential hazards of scrap processing.

9:55 AM

Transferring Molten Aluminum Safely: *Jake Niedling*[1]; [1]Alcoa Inc

A significant safety risk to employees occurs when molten aluminum is not handled properly. A large number of transfer related explosions reported every year is related to improper preparation or checks of the equipment receiving the molten aluminum. This applies to tapping smelters, crucibles, transfer launders, drain pans, hand tools and furnace tap equipment. It is important to have written procedures which cover the safety aspects of handling molten aluminum and emergency situations. Common solutions which minimize the safety risks will be reviewed for each process.

10:20 AM

Cause and Prevention of Explosions Involving DC Casting of Aluminum Extrusion Ingot: *Martin Ekenes*[1]; Ray Richter[2]; [1]Consultant; [2]Alcoa Inc

Explosions involving molten metal in aluminum DC casting operations are preventable. Accurate identification of root causes is critical to preventing such explosions. Incident reports of molten metal explosions submitted to the Aluminum Association since 1980 were analyzed to identify root causes of explosions in production of aluminum extrusion ingot during three stages of casting, "cast start", "steady state", and "cast end". From this analysis, suggestions for improving extrusion ingot casting safety are made. This paper is a companion to a previous paper, "Cause and Prevention of Explosions Involving DC Casting of Aluminum Sheet Ingot", *Light Metals 2005*.

10:45 AM Break

11:10 AM

Emerging Issues for PPE Programs and Management: Two Case Studies in PPE Program Review and Overhaul: *Charles Johnson*[1]; Robert Brewer[2]; [1]The Aluminum Association; [2]Steel Grip, Inc.

The goal of this research is to outline the common steps in a comprehensive review of a PPE program and to identify new and emerging issues in this field. Two cases are presented in which PPE programs at separate aluminum production facilities were overhauled. Interviews with the EH&S program directors responsible for the review and update of their PPE programs are compared with a general discussion of recent trends in the field. A list of issues such as pertinent regulatory requirements, industry best practices and guidelines, is presented. New options such as full laundering and contracted management of PPE systemsare discussed.

11:35 AM

Training for Preventing Molten Metal Explosions in Aluminum Cast Houses: *Martin Ekenes*[1]; [1]Consultant

A significant understanding of conditions leading to molten aluminum explosions has been gleaned through decades of industry research and incident investigations. However, the challenge remains how this understanding can be better utilized to reduce and ultimately eliminate molten metal explosions in aluminum casting operations. This paper describes training essential to achieving this worthy objective. Factors key to making training bear fruit in the cast house are also discussed.

12:00 PM Panel Discussion

Characterization of Minerals, Metals, and Materials: Characterization of Processing of Materials II

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division, TMS: Materials Characterization Committee
Program Organizers: Arun Gokhale, Georgia Institute of Technology; Jian Li, Natural Resources Canada; Toru Okabe, University of Tokyo

Thursday AM Room: Oceanic 8
March 1, 2007 Location: Dolphin Hotel

Session Chairs: Jiann-Yang Hwang, Michigan Technological University; Tetsuya Uda, Kyoto University

9:00 AM
Reduction of Titanium Oxide to Titanium Alloy by Hydrogen: *Hidehiro Sekimoto*[1]; Ryosuke Shioi[1]; Tetsuya Uda[1]; Yasuhiro Awakura[1]; [1]Kyoto University

It is very difficult to reduce titanium oxide to its metallic state because the affinity between titanium and oxygen is quite strong. Thus, the industrial titanium production process is a highly energy-consuming process and increases the titanium production cost. On the other hand, the significant portion of titanium is used as commercial alloys. We thus propose a new inexpensive route for the reduction of titanium oxide to titanium alloy. The chemical potential of titanium in alloy is largely lower when the affinity between titanium and an alloying element is strong. Consequently, even weaker reductant can reduce titanium oxide to the alloy. For example, hydrogen can not reduce titanium oxide to pure titanium metal but can reduce titanium oxide to titanium alloy; this is the case for Ti-Pt alloy. We will discuss the feasibility of such a process for Ti-Ni alloy with some experimental results and thermodynamic consideration.

9:20 AM
A Study on Electro-Magnetism of Peg-20000 Doped with Nano-Cobalt Ferrite Oxide Powder Containing La3+: *Xiao Li*[1]; [1]Central South University

Three kinds of nanometer magnetic particles, nano-cobalt ferrite oxide powders and those doped by LaCl3.nH2O with different ratio were prepared by sol-gel method. TG/DTG was applied for investigating thermo-decomposition process of the precursors, which showed that the activation energies of these particles were different in different stage, even not in the same stage for different sample. It has been showed that the magnetic particles with the average diameter less than 100nm were characterized by XRD and TEM. It indicated that the cobalt ferrite doped with La3+ affected its saturation magnetization and coercive force. The three kinds of nanometer magnetic particles were doped into polymer electrolyte peg-20000 with different rations respectively to obtain the compound substance with optimal conductivity.

9:40 AM
The Leaching Behavior of Heavy Metals in MSWI Bottom Ash by Carbonation Reaction with Different Water Content: *Nam-Il Um*[1]; Kwang-Suk You[1]; Gi-Chun Han[1]; Im-Chang Lee[1]; Kye-Hong Cho[1]; Ji-Whan Ahn[1]; Hee-Chan Cho[2]; [1]Korea Institute of Geoscience and Mineral Resources; [2]Seoul National University

The bottom ash is the residue generated during the incineration of municipal solid waste. The bottom ash mainly consists of glass, ceramics, ferrous metals, slags and non-ferrous metals such as aluminum. For recycling of the bottom ash, it must be stabilized by treatment process such as physical treatment and chemical treatment. Carbonation is one of pre-treatment that has been investigated by many researchers, recently. Most of carbonation process had been studied as a high water content(over 100%). But we have carried out the carbonation process under a various water content. In this study, the leaching behavior of heavy metals from municipal solid waste incineration bottom ash by carbonation process with different water content was investigated. As a result of a carbonation reaction utilizing a low(about 30%) and high(about 100%) water content, the heavy metals had various tendency about change of leaching behavior.

10:00 AM
Thermodynamic Measurement for Cr-P Alloy and Phosphorus Oxide with Double Knudsen Cell Mass Spectrometry: *Takashi Nagai*[1]; Masao Miyake[1]; Hisao Kimura[1]; Masafumi Maeda[1]; [1]University of Tokyo

Thermodynamic information on alloys and oxides forms a scientific foundation for the development of new technologies for refining steel and alloys, and also for the development of new materials with required physicochemical properties. In this research, the vapor pressure of phosphorus in equilibrium with a mixture of elemental Cr and Cr_3P at 1523 – 1623 K was directly measured by double Knudsen cell mass spectrometry with Cu-P alloy as a reference substance. The free energy of formation of Cr_3P was determined from the P_2 pressure. In addition, the thermodynamic properties of phosphorus oxide in a flux were measured by the double Knudsen cell mass spectrometry with a mixture of $Cr/Cr_3P/Cr_2O_3$ as a reference substance.

10:20 AM
High Pressure Assisted Sintering of Nanostructured Superhard Material: *Ana Lucia Skury*[1]; Humberto Cesar Vilela[1]; Sergio Monteiro[1]; [1]Universidade Estadual do Norte Fluminense

The development of nanostructured composites with improved physical and mechanical properties is in constant expansion in many areas of scientific and technological interst. One of these areas is that of superhard materials associated with the production of tools, such as those for drilling, wich are indispensable in petroleum exploration. The objective of this work was to develop a superhard nanocomposite based on CaCO3-Diamond-WC by means of high pressure and high temperature sintering. A mixture of powders of these components was initially submitted to high energiy ball milling and then sintered at 6GPa and 1400C. The results indicated that sintering time does not have a relevant influence on the density of the nanocomposites. The characterization by SEM revealed that the presence of CaCO3 significant contributes to the mechanism of diamond-WC nanoparticules consolidation. This results in a consistent nanostructured composite material.

10:40 AM Break

11:00 AM
Mineralogical and Crystallographic Characterization of Analcime Tuff from Jovici Deposit, Bosnia and Herzegovina: *Jovica Stojanovic*[1]; Ana Radosavljevic-Mihajlovic[2]; Slobodan Radosavljevic[1]; [1]Institute for Technology of Nuclear and Other Mineral Raw Materials; [2]Institute of Nuclear Science Vinca

The mineralogical and petrographical properties of the zeolitic tuff from Jovici deposit (Bosnia and Herzegovina) have been investigated. The samples rich in a natural analcime were characterized by microscopic, DTA/TGA, SEM and XRPD analyses. The Rietveld method was used for a quantitative phase determination. A zeolites are group of natural and artificial inorganic compounds, which have specific physical-chemical properties appropriate for industrial application. These minerals make specific group of alumosilicates within tectosilicates due to their origin, chemical compositions, and structural characteristics. A mineralogical composition of the zeolitic tuff consist of a: analcime, quartz, feldspars, mica, carbonates, volcanic glass, zircon, apatite, rutile, and plant fossils. The most abundant mineral is analcime, and the trapezohedral crystal forms are common. The analcime tuff sample was refined on cubic (Ia3d), tetragonal (I41/acd) and orthorhombic (Ibca) analcime unit-cell parameters. Tetragonal unit-cell parameters of analcime yielded the best refinement agreement factors.

11:20 AM
Effect of Additives on the Reaction of Carbothermal Reduction and Nitride Preparing for Vanadium Carbide Nitride: *Sansan Yu*[1]; Nianxin Fu[1]; Z.T. Sui[1]; [1]Northeastern University

In this paper, the producing process of using V2O3 as raw material to obtain vanadium carbide Nitride was analyzed through the means of thermodynamic. The analysis identified that conversion abide by the principle of reduction step by step in the process of conversion of V2O3. Effect of additives (such as Fe, compounds of alkaline earths and rare earths) and additive content on the nitrogen content of vanadium carbide nitride was studied. Experimental observations showed that additives can increase the nitrogen content of VCN. However, the effect on the nitrogen content caused by various of additives is different. Among the additives used in this paper, the effect of Fe and CaCO3 are verified the best and Fe can increased product density.

11:40 AM

Structural Modification in Graphite Treated at High Pressure and High Temperature: *Ana Lucia Skury*[1]; Rosane Manhaes[1]; Sergio Monteiro[1]; Angélica Santos[1]; [1]Universidade Estadual do Norte Fluminense

In recent investigation it was found that the association of zinc with a conventional system of graphite and catlyst alloy, used to produce diamond at high pressure and high pressure conditions, promotes an increase in synthesis productivity. The mechanism by zinc affects the nucleation of diamond crystals is still open discussion. In terms of diamond nucleation it is well known that size of the graphite crystallites influences the degree of diamond transformation. The present work studied the influence of zinc on the structural parameters of graphite treated at 4,5 GPa and 1300C, in contat with Ni-Mn as catalyst alloy. The results indicate that zinc greatly improves the catalystic action for the growth of crystallites. It was also found that the larger the amount of zinc, the larger the size of the crystallites. Beyond 8% of the zinc content in the reaction zone no diamond was formed.

12:00 PM

Thermodynamic Analysis on Preparation of Special Copper Precursor Powders with Oxalate Precipitation Process: *Youqi Fan*[1]; Chuanfu Zhang[1]; Jing Zhan[1]; Jianhui Wu[1]; [1]Central South University

According to the principles of simultaneous equilibrium and mass balance, a series of thermodynamic equilibrium equations of Cu^{2+}-$C_2O_4^{2-}$-NH_3-NH_4^+-H_2O system at ambient temperature are deduced theoretically and the logarithm concentration versus pH ($lg[Cu^{2+}]_T$ -pH) diagrams at different solution compositions are drawn. The results show that when pH is below 5.0, copper ion reacts with $C_2O_4^{2-}$ directly and the morphology of copper precursor powder is of pie-shape; When pH is above 5.0, copper ion coordinate with ammonia, the precipitation proceeds slowly accompanying with the release of copper ions from the multi-coordinated $Cu(NH_3)_n^{2+}$(n = 1 , 2 , 3, 4, 5). The morphologies of copper precursor powders are respectively spindle shaped aggregate (when $5.0 \leq pH \leq 8.0$) and of rod-shape(when $pH \geq 8.0$); Some experiments were made to confirm the relation between the total concentration of copper ion and pH. It is shown that the thermodynamic mathematical model is correct and the calculated values are basically accurate.

12:20 PM

The Effect of Mg Content in Limestone Ore on Characteristics of Precipitated Calcium Carbonate Powder: *Jung-Ah Kim*[1]; Ji-Whan Ahn[1]; Hwan Kim[2]; [1]Korea Institute of Geoscience and Mineral Resources; [2]Seoul National University

Synthesis of precipitated calcium carbonate (PCC) powder using limestone ore makes a large profit such as efficient development of resources and curtailment of import dependence. The first step for this is selection of suitable limestone ore to synthesis of PCC powder. In the synthesis research of PCC powder using reagent, it has been clarified by many researchers that attaching a little Mg ion has a good influence on synthesis of aragonite PCC powder. In this study, we thought about not Mg ion in synthesizing process but Mg ion in limestone ore (raw material. So the effect of Mg content in limestone ore on PCC powder characteristics was investigated. And shape of PCC powder transformed by change of Mg content in limestone ore.

Computational Thermodynamics and Phase Transformations: Modeling of Phase Transformations II

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: Corbett Battaile, Sandia National Laboratories; James Morris, Oak Ridge National Laboratory

Thursday AM — Room: Europe 11
March 1, 2007 — Location: Dolphin Hotel

Session Chair: Peter Voorhees, Northwestern University

9:00 AM

Assessments of the Phase Stability of the Al-Mg-B Alloys Using the CALPHAD Method: *Sungtae Kim*[1]; Donald Stone[1]; Jae-Ik Cho[2]; Jung-Chan Bae[2]; Chang-Seog Kang[2]; Joon Sik Park[2]; Chang-Yeol Jeong[2]; [1]University of Wisconsin; [2]Korea Institute of Industrial Technology

The in-situ composite based on the Al-Mg alloy matrix and the $(Al,Mg)B_2$ reinforcement compound phase has been investigated to develop for transportation equipment use, because it can reduce weight and thereby improve fuel efficiency. The suitability of a system for any particular application can be determined by microstructure of the alloy system, which is related to phase stability. In order to relate the thermodynamic properties of intermediate phases in the Al-Mg-B system to the phase stability, the binary Al-B and Mg-B and the ternary Al-Mg-B systems have been investigated. Based on updated thermodynamic properties, the phase stability of the Al-Mg-B system is assessed using the CALPHAD method. The financial support of the Korea Institute of Industrial Technology is gratefully acknowledged.

9:20 AM

Phase Stability in 409 Ferritic Stainless Steel at Elevated Temperatures: *Omer Dogan*[1]; Paul Jablonski[1]; [1]National Energy Technology Laboratory

Inexpensive stainless steels such as 409 ferritic steel is considered for use in parts of heat exchangers for solid oxide fuel cell applications. Thermodynamic calculations predict formation of austenite above 800°C, reaching to its maximum volume fraction of approximately 0.5 at about 1000°C. Experiments were conducted to investigate this predicted transformation from ferrite to austenite. Dilatometry was used to show that isothermal heat treatment is necessary for the transformation to take place. In addition to dilatometry, x-ray diffraction, and microscopy were utilized to quantify the transformation kinetics.

9:40 AM

Phase Transformations and Thermodynamic Modeling of the Cobalt-Titanium-Tin system.: *Jean-Claude Tedenac*[1]; Fucheng Yin[1]; Franck Gascoin[1]; [1]LPMC-Universite de Montpellier 2

The Ti-Sn alloy is a potential material for transient liquid phase (TLP) bonding which is used widely in the field of electronic components because of the low bonding temperature and high thermal stability [1]. In the ternary system Co-Ti-Sn two intermetallic compounds are present: CoTiSn (Heusler phase) and Co2TiSn (semi-heusler phase). The phase diagram and thermodynamic properties of the alloy system are of great value to alloy design and processing. A serie investigation of Ti-Sn based alloys, the thermodynamic assessment and calculation of Ti-Sn binary and Ti-Co-Sn ternary system are carried out in present work by means of the CALPHAD technique.

10:00 AM

Thermodynamic Modeling of the Ca-Ga-N System: *Wenxia Yuan*[1]; Gang Wang[2]; Jingfang Wang[1]; Zuofei Cai[1]; [1]University of Science and Technology Beijing; [2]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences

The growth of bulk GaN crystals has been proven to be a very challenging task because of the decomposition at high temperatures and the high melting

point of GaN. Adding the fluxs can grow the GaN single crystals successfully under mild experimental conditions. The knowledge about the phase diagrams and the thermodynamic properties of GaN with the flux Ca is essential to the growth process. Thermodynamic modeling of the Ca-Ga system was carried out based on available experimental phase diagram and thermodynamic data in the literature. As little information concerning phase diagram and thermochemical data involving in the region of Ca3N2-N was found in the literature, the Ca-N system was simplified as the Ca-Ca3N2 system. Combined with the Ga-N system modeled in the literature, the isothermal phase diagram of the ternary Ca-Ga-N system at 800°C was obtained.

10:20 AM
Linking Thermodynamics, Structure and Viscosity of Alumo- and Borosilicate Melts: *A. Grundy*[1]; [1]Centre for Research in Computational Thermochemistry, École Polytechnique de Montréal

Although amorphous silicates are common, and of significant technological importance, the complex interactions between its structure and its thermodynamic, transport and mechanical properties are still poorly understood. Over the past several years, through critical evaluation of all available thermodynamic and phase equilibrium data, we have developed a quantitative thermodynamic description of SiO_2-Al_2O_3-B_2O_3-MgO-CaO-FeO-Fe_2O_3-ZnO-MnO-PbO melts using the Modified Quasichemical Model for short-range ordering. From the resultant database, we can calculate the local structure of the liquid, in terms of the bridging behavior of oxygen, as a function of composition and temperature. In the present work a model is developed relating this local structure to the viscosity. Based only on parameters obtained by fitting viscosity data for unary and binary sub-systems, the model permits reliable prediction of viscosities of multicomponent melts.

10:40 AM
Application of the Cluster/Site Approximation (CSA) to the FCC Phases in NI-AL-CR-PT System: *Jun Zhu*[1]; Weisheng Cao[1]; Ying Yang[2]; Y. Chang[1]; [1]University of Wisconsin; [2]CompuTherm LLC

We present a thermodynamic description of Ni-Al-Cr-Pt with the fcc phases modeled by the CSA instead of the Bragg-Williams Approximation and the description of the remaining phases adopted from known descriptions of Ni-Al-Cr, Cr-Pt, and a preliminary description of Ni-Al-Pt. The CSA was used for two reasons: (i) it considers the existence of short range order (SRO), yet retains computational advantage over the CVM and (ii) experimental data are sparse. Past experience demonstrated that fewer parameters are needed when using the CSA instead of the Bragg-Williams Approximations. Descriptions of the Ni-Cr-Pt, Al-Cr-Pt, and Ni-Al-Pt were obtained by extrapolation but slight modeling was done for Ni-Al-Pt using limited experimental data. We believe this description can be used for practical applications at the moment but more importantly, the model-calculated phase diagrams can be used to identify limited number of alloys for experimentation, rapidly yielding a reliable description.

11:00 AM Break

11:20 AM Invited
Coarsening in Morphologically Complex Systems Following Spinodal Decomposition: Y. Kwon[1]; K. Thornton[2]; *Peter Voorhees*[1]; [1]Northwestern University; [2]University of Michigan

Nature frequently produces two-phase mixtures with great morphological complexity, such as the bicontinuous interfaces found following spinodal decomposition. Through large-scale computer simulations we have examined the evolution of the three-dimensional interfacial morphology following spinodal decomposition for both critical and off-critical quenches. We characterize the morphology of the resulting interfaces using the probability of finding a patch of interface with a pair of principle curvatures, the interfacial shape distribution, and the topology of the interfaces using the genus. In two dimensions off-critical quenches, where the volume fractions of each phase are not equal, very quickly result in an array of particles. In contrast, in three-dimensions over a wide range of volume fractions the interfaces remain bicontinuous over very long coarsening times. We find that the morphology of the interfaces is different from those of the critical quenches but the topology of the interfaces is very similar.

11:50 AM
Precipitation Simulation of fcc Iron Precipitates in Cu-Fe Alloys: María del Carmen Gutierrez-Mendez[1]; Erika Avila-Davila[1]; *Victor Lopez-Hirata*[1]; Viridiana Melo-Maximo[1]; Maribel Saucedo Muñoz[1]; [1]Instituto Politecnico Nacional

This study shows the numerical simulation of the fcc-Fe precipitation in a Cu-rich Cu-Fe alloys after aging at temperatures of 673, 773 and 823 K for different times. The numerical simulation was based on the solution of the non-linear Cahn Hilliard equation by the finite difference method. The results of the microstructural simulation indicated that the formation of fcc-Fe precipitates occurred by the nucleation and growth mechanism. The morphology of Fe precipitates was plate-like at the early stages of aging and changed to a round shape for more prolonged agings. The size of precipitates and its kinetics growth increased as the aging time and temperature increased. The simulation microctuctural evolution of the fcc-Fe precipitates in the Cu-rich matrix showed a good agreement with the experimental results obtained by the field ion microscope analysis of the same composition alloy after aging at the same conditions.

12:10 PM
Molecular Dynamics and Phase Field Modeling of Pressure-Driven Solidification: *James Belak*[1]; James Glosli[1]; Patrice Turchi[1]; Mehul Patel[1]; Fred Streitz[1]; [1]Lawrence Livermore National Laboratory

Large parallel computers have enabled MD simulations of pressure-driven solidification of sufficient scale to observe the formation of realistic microstructure.[1] Here, we analyze these simulations to extract nucleation and growth rates and information necessary to validate phase-field models. We calculate the coarse-grained phase-field order parameter from the local atomic coordinates and use the MD to drive the evolution of the phase field. The relevant interfacial mobility and energy follows directly from the atomistic dynamics. We also calculate x-ray scattering from the nucleating and evolving microstructure as a guide to future in situ experiments at fourth generation x-ray light sources. [1]F. H. Streitz, J. N. Glosli, and M. V. Patel, "Beyond Finite-Size Scaling in Solidification Simulations," Phys. Rev. Lett. 96, 225701 (2006). This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

12:30 PM
Numerical Simulation of High Temperature Air Combustion: Yuan Ling[1]; Zhu Miao-Yong[1]; [1]Northeastern University

High temperature air combustion (HTAC) is one of the most important innovations in the field of combustion and heat engineering. Based on commercial software STAR-CD, the combustion process using converter gas as fuel is numerical simulated. The influences of preheating temperature and gas-flow rate on combustion are studied. The influences of different fuel component on temperature field are analyzed.

Computational Thermodynamics and Phase Transformations: Nanomaterials and Confined Systems II

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: Corbett Battaile, Sandia National Laboratories; James Morris, Oak Ridge National Laboratory

Thursday AM Room: Europe 10
March 1, 2007 Location: Dolphin Hotel

Session Chair: Corbett Battaile, Sandia National Laboratories

9:00 AM Invited
Phase Equilibria and Concentration Profiles in Nanoscale Binary Alloys: *Jeffrey Hoyt*[1]; [1]Sandia National Laboratories

Phase equilibrium behavior in nanoscale systems is often quite different from the bulk counterpart. In this work molecular dynamics and Monte Carlo simulations have been used to study equilibrium in nano-size liquid droplets of Cu-Pb alloys and the results demonstrate that the concentration profile through the spherical particles is decidedly non-uniform. The concentration profile is a direct result of the lower surface tension of liquid Pb relative to that of Cu and the non-uniformity can be modeled using the Cahn-Hilliard description of alloy thermodynamics. The modeling procedure provides an estimate of the gradient energy coefficient. In addition, the surface segregation tendency and the small system size are shown to alter the conditions for solid-liquid equilibrium and the shifts of the solidus and liquidus curves, relative to the bulk system, will be presented.

9:30 AM
Molecular Dynamics Simulations of Multiple Twinned Ag Nanowires: *Joshua Monk*[1]; Jeff Hoyt[2]; Diana Farkas[1]; [1]Virginia Tech; [2]Sandia National Laboratory

Nano scale wires and particles often exhibit a multiple twinned structure. In particular, Yacaman and co-workers have shown that nanowires of Ag, produced by the polyol reduction of AgNO3, grow along a <110 > type crystallographic direction and have a pentagonal cross section with five {111} twins connecting the wire center to the corners of the pentagon. In this work we use molecular dynamics simulations with embedded atom method (EAM) interatomic potentials for Ag to compute the ground state energies as a function of size for both the multiple twinned structure and the bulk equilibrium crystal shape as determined from a Wulff construction. A comparison of the two energies provides an estimate of the crossover size below which the multiple twinned structure is stable. Various contributions to the total energy, such as elastic strain energy, twin boundary energy and surface energies, are discussed.

9:50 AM
Simulation on the Phase Transformation of Silicon under Multiaxial Stress: *Seongmin Jeong*[1]; Yoshitaka Umeno[1]; Takayuki Kitamura[1]; [1]Kyoto University

Silicon undergoes a series of phase transformations under simple mechanical test or treatments, such as nanoindentation or grinding. In the most real cases, complex stress rather than pure uniaxial stress applies the testing materials. Moreover, crystal structure of silicon shows anisotropic behavior, which makes it difficult to analyze the stress analysis for the phase transformation of silicon. These difficulties are the reason why the transformation mechanism under indentation has still been studied, but clearly understood yet. Therefore, in this study, we conducted calculations on the critical stress level on the phase transformation of silicon under multi-axial stress. Molecular dynamics simulation for very simplified model was conducted to obtain ideal critical stress for phase transformation. Moreover, in order to predict the phase distributions under complex stress state, shear stress effect on the phase transformation was also conducted.

10:10 AM Break

10:30 AM Invited
Control of Melting Using Nanoscale Coatings: *Kerwyn Huang*[1]; Tairan Wang[2]; John Joannopoulos[3]; [1]Princeton University; [2]Omniguide Communications; [3]Massachusetts Insitute of Technology

We present ab-initio density-functional simulations of the state of several semiconductor surfaces at temperatures near the bulk melting temperatures. We find that the solid-liquid phase-transition temperature at the surface can be altered via a microscopic (single-monolayer) coating. Our results show that a single-monolayer GaAs coating on a Ge(110) surface above the Ge melting temperature can dramatically reduce the diffusion coefficient of the Germanium atoms, going so far as to prevent melting of the bulk layers on the 10ps time scale. In contrast, a single-monolayer coating of Ge on a GaAs(110) surface introduces defects into the bulk and induces melting of the top layer of GaAs atoms 300 K below the GaAs melting point. In addition, we suggest that the Ge monolayer causes the GaAs(110) surface to melt through transient penetration of the Ge atoms into the bulk, which locally initiates the collective diffusive motion of large groups of Ga/As atoms.

11:00 AM
A New Polymorph of Zinc Oxide in Nanowires under Tensile Loading: *Ambarish Kulkarni*[1]; Min Zhou[1]; Kanoknan Sarasmak[2]; Sukit Limpijumnong[2]; [1]Georgia Institute of Technology; [2]Suranaree University of Technology

We report a previously unknown reversible phase transformation from the wurtzite structure to a 5-fold coordinated graphitic structure in ZnO nanowires. Molecular dynamics simulations show that this transformation occurs in [01-10]-oriented nanowires under uniaxial tensile loading and is associated with recoverable strains up to 15% and a low level of hysteretic energy dissipation (0.16 J/m^3) per transformation cycle. First principles calculations show that this new polymorph (herein denoted as HX) corresponds to a distinct minimum on the enthalpy surfaces of ZnO under the conditions of the uniaxial tensile stress considered. The slender one-dimensional shape of the nanowires and the uniaxial nature of the tensile loading along the [01-10] crystalline direction combine to provide the necessary driving force for this transformation which occurs through atomic shifts toward higher coordination and ionicity.

11:20 AM
Surface Stress and Relaxation in Nanoscale Electrodes and Clusters: Response to Electric Charging: *Jörg Weissmüller*[1]; Florian Weigend[2]; Ferdinand Evers[2]; Raghavan Viswanath[3]; Dominik Kramer[3]; [1]Forschungszentrum Karlsruhe and Universitaet des Saarlandes; [2]Forschungszentrum Karlsruhe and Universitaet Karlsruhe; [3]Forschungszentrum Karlsruhe

Surface forces have important consequences for equilibrium states in nanomaterials. Recent experiments reveal a large macroscopic expansion or contraction of nanoporous metals, a response to varying surface stress, when their interface with electrolytes is electrically polarized. This raises the questions: which microscopic processes relate the surface forces to relaxation, electronic structure, and bonding at a charged surface, and what is the role of surface chemistry? We compare experiments on nanoporous platinum [Weissmüller et al., Science_300(2003)312.] and gold [Kramer et al., Nano_ Lett_4(2004)793.] electrodes to numerical results from density-functional theory (DFT) of atomic relaxation in 309 atom gold cluster ions in vacuum [Weigend et al., Small_(2006)_in_press]. Amazingly, the cluster responds to charging consistently with a continuum model extrapolating experimental observations to extremely small size. Based on the insights from DFT and experiment we propose a microscopic model for surface stress and relaxation at charged metal surfaces, which explains the most important trends.

11:40 AM
Symmetry Breaking and Spatial Ordering in Stress-Induced Surface Self-Assembly: *Yanfei Gao*[1]; [1]University of Tennessee

For a class of problems of self-assembled nanostructures on solid surfaces, the long range spatial ordering is critically dependent on the anisotropy. Examples include self-organization in phase-separating monolayer, quantum dot growth, and surface roughness evolution of a stressed solid during chemical etching. Using linear and nonlinear perturbation theories, this presentation gives a complete analysis of this orientation dependence on parameters that represent the anisotropy in applied stress (or misfit stress, surface stress, etc.), elasticity stiffness and surface energy. A universal formulation is developed to examine the energetically favored orientation of those self-assembled structures. The

Stroh formalism is employed in this formulation to treat arbitrary elasticity anisotropy in a half-space and in a multilayer substrate.

12:00 PM

Molecular Dynamics Simulations of the Role of Adatoms, Interstitials, and Grain Boundaries in Thin Film Stress Evolution: Stephen Foiles[1]; *Edmund Webb*[1]; Chun-Wei Pao[1]; David Srolovitz[2]; Jerrold Floro[1]; [1]Sandia National Laboratories; [2]Yeshiva University

To investigate stress generation mechanisms during thin film growth, simulations were performed of the interaction between interstitial atoms and a Sigma 79 tilt grain boundary (GB) in Ni. One theory asserts that interstitials, trapped during deposition due to kinetic effects, generate compressive stress during thin film growth; it has also been asserted that GBs may assist interstitial incorporation. Simulation results will be presented demonstrating that, both far from and near to a free surface, interstitial formation energy is greatly reduced for normal distances within 1 nm of the GB. Proximity to a free surface changes results only in that some percentage of interstitials formed in the surface plane equilibrate into adatom positions. Simulations of deposition onto a Ni(111) surface intersected by sigma 79 GBs demonstrate that adatoms are readily incorporated into the GB, generating compressive stress with a magnitude dependent upon grain size.

Dynamic Behavior of Materials: Fracture

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

Program Organizers: Marc Meyers, University of California; Ellen Cerreta, Los Alamos National Laboratory; George Gray, Los Alamos National Laboratory; Naresh Thadhani, Georgia Institute of Technology; Kenneth Vecchio, University of California

Thursday AM Room: Europe 3
March 1, 2007 Location: Dolphin Hotel

Session Chairs: Naresh Thadhani, Georgia Institute of Technology; Ellen Cerreta, Los Alamos National Laboratory

9:00 AM Invited

Molecular Dynamics Simulation of Dynamic Damage and Failure of Materials: *Wenjun Zhu*[1]; Wenqiang Wang[1]; Zhengfei Song[1]; Xiaoliang Deng[1]; Hongliang He[1]; [1]Institute of Fluid Physics

The characteristic length scale of dynamic damage and failure of materials extends from atomistic-scale to macro-scale. Molecular Dynamics (MD) simulation plays a critical role to understand microstructure evolution, dynamic damage and failure in materials. Due to limitation of calculation, MD simulation usually deals with incipient process of dynamic damage at nano-scale. In this topic, we present two progresses in MD simulation of dynamic damage and failure, where one is that lattice orientation effect to nano-void growth in copper under shock loading by classical MD simulation, another is that a unusual oscillating crack propagation in rubber sheet under biaxial tension by MD simulation in general sense (Lattice Model) at macro-scale with consideration of unique mechanical properties of rubber: hyperelasticity, viscoelasticity and nonlocal elasticity. These results as example shed light to develop mutiscale modeling method to describe and deeply understand dynamic damage and failure of materials.

9:30 AM

D3 in Armor Ceramics: Defects, Deformation and Damage at High Strain Rates: *James McCauley*[1]; [1]Army Research Laboratory

In order to simulate the performance of structural ceramics in high strain rate/high compressive stress environments it is critical to quantify the various micromechanisms and physics of deformation, damage accumulation and failure. The crystallographic and microstructural controlled mechanisms, including the role of defects, which influence their behavior in dynamic environments is not that clear in most cases. This presentation will describe recent results concerning defect characterization in SiC armor material, HREM characterization of B4C from ballistic impact experiments, alumina from plate impact experiments and AlON from Edge-on Impact and Kolsky bar experiments. The work resulted from collaborations with K.T. Ramesh, Mingwei Chen and Bhasker Paliwal of Johns Hopkins, Victor Greenhut, Mike Bakas, Richard Haber and Dale Niesz of Rutgers, Neil Bourne of the University of Manchester, UK, George Quinn, NIST, Elmar Strassburger of the Ernst Mach Institute, Germany and Datta Dandekar and Parimal Patel of the Army Research Laboratory.

9:45 AM

Validating Theories for Brittle Damage: *Rebecca Brannon*[1]; Joseph Wells[2]; [1]Sandia National Laboratories; [2]JMW Associates

Comparing simulated predictions of internal damage against high resolution diagnostic visualizations (as available from X-ray computed tomography, XCT) is preferable to simply assessing a model's ability to predict penetration depth, especially if one hopes to perform subsequent "second strike" analyses. We present results of a study in which crack networks are seeded by using a statistically perturbed strength whose median is inherited from a deterministic "smeared damage" model with adjustments to reflect experimentally established size effects. This minor alteration of an otherwise conventional damage model dramatically mitigates mesh dependencies and produces (at virtually no computational cost) far more realistic cracking patterns that are well suited to XCT validation. For Brazilian, spall, and indentation tests, simulations will be shown to correlate well with data. Potential for more stringent sub-surface XCT validation of these simulations will be discussed.

10:00 AM

Wiebull Analysis of Variability in Dynamic HEL and Spall Properties of Tantalum: *Michael Furnish*[1]; William Reinhart[1]; Wayne Trott[1]; Lalit Chhabildas[1]; Tracy Vogler[1]; [1]Sandia National Laboratories

Two suites of impact experiments utilizing spatially-resolved velocimetry have been conducted to assess spatial variability in dynamic yield properties of tantalum. Samples in the first suite had a uniform refined ~ 20 micron grain structure with a strong axisymmetric [111] crystallographic texture. In the second suite the grain size was ~45 microns. Weibull failure analysis methods were used to assess variability of the Hugoniot Elastic Limit and spall. Spallation of the larger-grain material yielded slightly greater beta values (12 – 14) than did that of the finer grain material (10 – 12). Yielding at the HEL yielded lower values (7 – 10) for beta, corresponding to greater spatial variability than observed for spallation. This is also reflected in gross features of the waveforms. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

10:15 AM

Advances in XCT Diagnostics of Ballistic Impact Damage: *Joseph Wells*[1]; Rebecca Brannon[2]; [1]JMW Associates; [2]Sandia National Laboratories

The relatively recent introduction of quantitative and volumetric X-ray computed tomography, XCT, ballistic impact damage diagnostics has made significant inroads in expanding our knowledge base of the morphological variants of physical impact damage. Yet, it appears that the current state of the art in computational and simulation modeling of ballistic performance remains predominantly focused on the penetration phenomenon without detailed consideration of the physical characteristics of actual impact damage. Similarly, armor ceramic material improvements appear more focused on penetration resistance than on improved intrinsic damage tolerance/ damage resistance. Basically, these approaches minimize our understanding of the potential influence that impact damage may play in the mitigation and/or prevention of ballistic penetration. Current capabilities of XCT characterization, quantification, and visualization of complex impact damage variants are demonstrated and discussed for impacted armor ceramic target materials. Potential benefits of incorporating such impact damage diagnostics in future computational modeling are also discussed.

10:30 AM Break

10:45 AM

Microstructural Effects in FCC Alloys after Small Charge Explosions: *Donato Firrao*[1]; Paolo Matteis[1]; Giorgio Scavino[1]; Graziano Ubertalli[1]; Maria Ienco[2]; Paolo Piccardo[2]; Maria Pinasco[2]; Enrica Stagno[2]; Girolamo Costanza[3]; Roberto Montanari[3]; Maria Tata[3]; Giovanni Brandimarte[4]; Santo Petralia[4]; [1]Politecnico Di Torino; [2]Università di Genova; [3]Università di Roma Tor Vergata; [4]Marina Militare Italiana

Effects on metal targets after an explosion include: fracture, plastic deformations, surface modifications, microstructural crystallographic alterations, with ensuing mechanical properties changes. In the case of small charge explosions, macroscopic effects are restricted to very small charge-to-target distances, whereas crystal alterations can still be observed at moderate distances. Microstructural variations, induced on gold alloy samples with two different grain sizes, as compared to already published results on AISI 304Cu steel samples, are illustrated. The samples were subjected to blast wave overpressures in the 0.5 to 195 MPa range. Minimum distances and peak pressures, which could still yield observable alterations, were especially investigated. Blast-related microstructural features were observed on exposed and perpendicular sections. X-ray diffraction analyses were performed to identify modifications of phase, dislocation density, frequency of mechanical twins and texture before and after explosions. Optical and scanning electron microscopy observations evidenced partial surface melting, zones with recrystallization phenomena, and mechanical twinning.

11:00 AM

The Investigation of the Ballistic Performance of Armor Ceramics against Long Rod Penetration: *Fenglei Huang*[1]; Liansheng Zhang[1]; [1]Beijing Institute of Technology

The quantitative evaluation and prediction of the ballistic performance of ceramics remain challenge because of the lack of the dynamic response of ceramics under impacting and penetration, especially with long-rod projectile. In this paper, a series of depth of penetration (DOP) tests have been carried out to investigate the influence of the ceramics thickness on the residual penetration and the general ballistic efficiency index - differential efficiency factor (DEF) . Based on the experimental results, an enhanced DEF is proposed which is independent of the ceramic thickness and structural effects. According to the new DEF equation, the parameters that affect the ballistic performance of the ceramics are the density, internal friction and compression strength in case of long-rod thick-tile-armor interaction. Therefore, the enhanced DEF is capable of evaluating the ballistic efficiency of ceramics against long rod penetration.

11:15 AM

Microstructure, Mechanical Property, and Ballistic Resistance Correlations of High-Strength, High-Toughness Steels: *Xian Zhang*[1]; Eric Focht[1]; Ernest Czyryca[1]; [1]Naval Surface Warfare Center

A study was conducted to examine correlations among microstructure, mechanical properties, and ballistic limit V50 for a low carbon, copper-strengthened alloy steel (HSLA-100) and a developmental low carbon 10% Ni steel. A broad range of heat treatments was carried out to obtain wide variations in microstructure and properties. 20 mm FSP ballistic tests were conducted to determine the V50, and the data were analyzed for correlations to variation in mechanical properties. A comprehensive microstructural characterization of the penetration features was made. It was found: (1) Only a weak correlation between tensile strength and V50 could be established, and other properties showed mixed results; (2) Adiabatic shear banding (ASB) formed in all ballistic test samples, but its type and formation mechanism were not strongly related to the variation of microstructure, especially the type of secondary precipitates; (3) The prior ASB dynamic global deformation played a determining role in ballistic limit (V50).

11:30 AM

Plate Impact Investigation of High-Speed Friction at Metal-on-Metal Interfaces: *Fuping Yuan*[1]; Vikas Prakash[1]; [1]Case Western Reserve University

In the present study plate-impact pressure-shear friction experiments were conducted to investigate the dynamic slip resistance and time-resolved growth of molten metal films during dry metal-on-metal slip under extreme interfacial conditions. By employing tribo-pairs comprising hard tool-steel against relatively low melt-point metals such as 7075-T6 aluminum alloy, interfacial friction stress of up to 300 MPa and slip speeds of approximately 250 m/s have been achieved. These relatively extreme interfacial conditions are conducive to the development of molten metal films at the tribo-pair interface. A Lagrangian finite element code is developed to understand the evolution of the thermo-mechanical fields and their relationship to the observed slip response. During the early part of friction slip the coefficient of kinetic friction is observed to decrease with increasing slip velocity. During the later part transition in interfacial slip occurs from dry metal-on-metal sliding to the formation of molten Al films at the tribo-pair interface.

11:45 AM

Spall Strength of Glass Fiber Reinforced Polymer Composites: *Fuping Yuan*[1]; Liren Tsai[1]; Vikas Prakash[1]; [1]Case Western Reserve University

In the present study, a series of plate impact experiments were performed on glass fiber reinforced polymer composites (ARL GRP & British GRP), with two different type of weaves, to investigate the spall (delamination) strength following normal shock compression and combined compression and shear wave loading. The measured spall strength, as a function of the applied shear strain and the normal stress, was used to develop a 3-dimensional failure surface for the two composites. The results indicate that the spall strength of the two GRP materials decrease with increasing compressive stress and shear stress levels. The results also indicate that the British GRP has much higher spall strength when compared to the ARL GRP. The maximum spall strength measured for British GRP was 119.5 MPa, while the maximum spall strength measured for ARL GRP was 53.7 MPa.

12:00 PM

Static and Dynamic Indentation Response of Fine Grained Boron Carbide: Dipankar Ghosh[1]; Spandan Maiti[1]; *Ghatu Subhash*[1]; [1]Michigan Technological University

Fine grained boron carbide ceramic was consolidated using plasma pressure compaction method. Static and dynamic indentations were conducted to determine strain rate sensitivity of hardness and fracture toughness as a function of grain size. The indentation-induced cracks during static indentation were transgranular in nature with crack orientation within each grain at an angle to the macroscopic crack direction. This zig-zag pattern is speculated to follow the cleavage planes in each grain. On the other hand, the induced cracks under dynamic indentations showed relatively straight crack facets. A fracture mechanics based finite element framework in conjunction with cohesive zone modeling is developed to model the observed crack pattern as a result of competition between fracture toughness and energetically favorable cleavage plane orientations. A parametric study of the effects of macroscopic crack orientation and cleavage plane strength on the crack propagation path will be presented.

12:15 PM

Dissimilar Dynamic Response of Two Nitinol Alloys: 50NiTi vs. 55NiTi (at.%): *Raghavendra Adharapurapu*[1]; Fengchun Jiang[1]; Kenneth Vecchio[1]; [1]University of California San Diego

While a combination of solution-treatment, cold-work and heat-treatment are necessary to optimize the properties of 50NiTi, superelasticity (SE) and shape memory (SM) in the Ni-rich 55NiTi was achieved from the same ingot by simple heat treatments only. The main difference between the two alloys is that Ni-Ti alloys with Ni content greater than 50.6 at.% are sensitive to heat treatment; aging in these materials leads to precipitation of several metastable phases. Effect of strain rate on these two Nitinol alloys was investigated in compressive and tensile loading conditions at 10^{-3}/s and 1200/s. The main observation is that the plateau that was clearly delineable in SE 50NiTi during quasi-static tensile testing disappeared at high-strain rates. Contrarily, the SE 55NiTi that exhibited a positive-slope plateau during QS tensile testing, exhibited a perfectly flat plateau during dynamic loading conditions. The relevant deformation mechanisms that lead to afore-mentioned dissimilar dynamic responses are discussed.

12:30 PM

Effect of Product Form on the Dynamic Response of 50NiTi: Sheet vs. Rod Textures: *Raghavendra Adharapurapu*[1]; Fengchun Jiang[1]; Kenneth Vecchio[1]; [1]University of California San Diego

There is a growing interest in exploring NiTi alloys for high-strain rate applications where NiTi may be in cylindrical, sheet, tube and even porous geometries. However, the response of NiTi is dependent on the product form through their respective textures and geometry. In the current work, we present

the dynamic response of NiTi in rod and sheet form between –196°C and 400°C under tensile loading at~1200/s. We further compare the dynamic results with corresponding behavior observed at quasi-static strain rates. The main results, presented in the form of stress at 0.2% (strain offset) vs. temperature, exhibit a three-stage character. A striking difference in the 0.2% stress at higher temperatures (stage III) were observed in both the products, where the yield strength remains nearly temperature independent under quasi-static loading between 100°C to 400°C; whereas it varies linearly with temperature under dynamic loading.

12:45 PM

Microstructural Effects on Plastic Deformation and Damage Nucleation in Shocked Cu Multicrystals: *Stephan DiGiacomo*[1]; Heber D'Armas[2]; Sheng-Nian Luo[3]; Scott Greenfield[3]; Pedro Peralta[1]; Manuel Parra Garcia[1]; [1]Arizona State University; [2]Universidad Simón Bolívar; [3]Los Alamos National Laboratory

Reliable predictions of material performance under dynamic loading require a thorough understanding of the deformation mechanisms leading to damage nucleation and failure. To further investigate these mechanisms, plate impact tests have been conducted on multicrystalline copper discs 200µm thick, 10mm in diameter. In-situ diagnostics such as velocity (VISAR) and displacement interferometry are being used to correlate the dynamic response of the samples following impact to damage present in recovered samples. Orientation Imaging Microscopy (OIM) is used to characterize thru-thickness and in-plane plastic deformation and lattice rotation in recovered samples. Damage nucleation and failure (spall) of recovered samples is being related to microstructural sites such as grain boundaries, pre-existing pososity, and triple-points.

Electrode Technology Symposium (formerly Carbon Technology): Cathode Part III: Titanium Diboride

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee
Program Organizers: John Johnson, RUSAL Engineering and Technological Center LLC; Morten Sorlie, Elkem Aluminium ANS

Thursday AM Room: Southern 3
March 1, 2007 Location: Dolphin Hotel

Session Chair: Elias Symphronio de Castro Neto, CBA - Companhia Brasileira de Alumínio

9:00 AM Introductory Comments

9:05 AM

Chemical Stability of Pitch-Based TiB_2–C Coatings on Carbon Cathodes: *M. Ibrahiem*[1]; T. Foosnæs[1]; H. Øye[1]; [1]Norwegian University of Science and Technology

The chemical stability of pitch-based TiB_2-C coated samples was studied. Results from unpolarized exposure to liquid aluminium showed that one hour of exposure time was not enough for aluminium to penetrate the sample. After 48 hrs, a penetration depth of 166 µm was reached through the open pores and grain boundaries. Some Al_4C_3 and Al_2O_3 formed at the aluminium coating interface as well as in the aluminium pool. Unpolarized exposure to electrolyte resulted in grain boundary corrosion and surface attack. Rutile (TiO_2) grains were noticed at the coating surface and inside the coating. Prolonged electrolysis experiments were carried out with respect to aluminium carbide formation. Aluminium carbide did not form at the coating-carbon interface at 100 hrs electrolysis. It formed locally at the surface and inside the coating. Pitch-based TiB_2-C coating acted as a sodium diffusion barrier. The wettability of the coating by the liquid aluminium during electrolysis is the key of the barrier action of the coating towards sodium and electrolyte.

9:30 AM

Application of TiB2-Coating Cathode Blocks Made by Vibration Molding for 300 kA Aluminum Reduction Cells: *Ren Bijun*[1]; Zhongning Shi[2]; Yungang Ban[2]; Songling Dai[1]; Zhaowen Wang[2]; Zhuxian Qiu[2]; [1]Yichuan Electric-Power and Aluminium Group; [2]Northeastern University

Some carbon cathode blocks surface coated with TiB2-C compound layer were made by vibration molding process for 300 kA aluminum reduction cells when the cells were relined in Yichuan aluminum smelter plant. Cathode voltage drops, electric resistance, titanium content in primary aluminum were detected on line after the cell startup. The cathode voltage drops of TiB2-coating(30-40wt% TiB2 content) was 261-286mV and the titanium content in primary aluminum was 0.0025wt%, while the average electric resistance was of 0.98µO. The results showed that TiB2 coating cathode blocks might save energy, improve the CE and prolong the cell lift time.

9:55 AM

Application of TiB2/C Composite Cathode Coating Solidified at Ambient Temperature in 300kA Prebaking Aluminium Reduction Cell: *Yungang Ban*[1]; Zhongning Shi[1]; Hongmin Kan[1]; Zhaowen Wang[1]; Zhuxian Qiu[1]; [1]College of Materials and Metallurgy

Introduced the technique of TiB2/C composite cathode coating solidified under ambient temperature and its industrial application results in the 300kA aluminium reduction cells are presented in this paper. The surface of the coating is smooth with no cracks and separate layers after 24 hours solidification and combined with cathode tightly. The operation of coating cells was improved to gain more uniform current distribution and lower anode cathode distance. There is a little change of cryolite ratio (CR) of electrolyte during cell startup, which will prorect cathode blocks from sodium penetration. The average ohmic drop of two test cells bottom was lessened by 9.5mV and 10.3mV after startup 6 months. The current efficiency of the two test cells was increased by about 0.68% and 0.81%. The period of validity of TiB2/C composite cathode coating can reach about 30 months. Obviously the TiB2/C coating can save energy and increase pot life.

10:20 AM

Preparation of TiB2 Inert Cathode by Electrodeposition Process for Aluminum Electrolysis: *Yungang Ban*[1]; Zhongning Shi[1]; Hongmin Kan[1]; Zhaowen Wang[1]; Zhuxian Qiu[1]; [1]College of Materials and Metallurgy, Northeast University

The TiB2 as inert cathode material for aluminum electrolysis, was electrodeposited successfully on graphite cathode as a coating by way of K2TiF6–KBF4–KF–KCl molten salts electrolysis at 820° for 4 hours with current density 0.3~0.5A/cm2, of which the composition of the electrolyte used is 15.3 K2TiF6, 24.2 KBF4, 53.1 KF, 7.4 KCl in % as mass fraction. XRD was used to detect the composition of the coating with the SEM used for morphology observation. The results indiated that the coating with a current density of 0.4A/cm2 is composed of simplex TiB2 with no impurity. The 0.2 mm thick TiB2 coating is smooth and appears silvery metallic luster, especially it is bonded firmly to the graphite substrate. The distribution of Ti element is well-proportioned. It is confirmed that Ti and B can be co-deposited to form TiB2 coating on graphite cathode surface as an inert cathode in this way.

10:45 AM

Sodium Expansion of Carbon/TiB2 Composite Cathodes during Aluminum Electrolysis: *Jilai Xue*[1]; Qingsheng Liu[1]; [1]University of Science and Technology

Experimental studies on sodium expansion of carbon/TiB2 composite cathodes were carried out during laboratory aluminum electrolysis. Numerical modeling was applied for this Na diffusion-expansion process. In general, the rate of Na expansion reduced with increasing TiB2 content in the carbons and with lowering cryolite ratio. Also the time for reaching Na saturation in the composite cathodes and the coefficient for the Na diffusion varied with the addition of TiB2.

11:10 AM
Study on Expansion of Tib2/C Compound Cathode and Sodium Penetration during Electrolysis: Wang Yaowu[1]; Feng Naixiang[1]; You Jing[1]; Peng Jianping[1]; Duan Xueliang[2]; Wu Jianguo[2]; *Ma Shaoxian*[3]; [1]Northeastern University; [2]Shanxi Jinyang Carbon Company, Ltd; [3]Northeastern University Design and Research Institute

The expansion of TiB2/C compound cathode during electrolysis was studied in laboratory. It was found that the expansion of TiB2/C compound cathode decreases with the increase of TiB2 content in TiB2/C. Na had the same penetration mechanism in TiB2/C cathode as that in normal carbon cathode. In TiB2/C cathode, Na not only penetrated into TiB2/C through pores, but also penetrated into TiB2/C through carbon grains inside TiB2/C cathode. Meanwhile, Na acted with carbon inside TiB2/C to produce compound among grains and hence led to grain expansion. It showed that there was linear relation between the depth of Na penetration of the TiB2/C cathode and √t.

Electrode Technology Symposium (formerly Carbon Technology): Rodding and Coke Inventory

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Aluminum Committee
Program Organizers: John Johnson, RUSAL Engineering and Technological Center LLC; Morten Sorlie, Elkem Aluminium ANS

Thursday AM Room: Southern 1
March 1, 2007 Location: Dolphin Hotel

Session Chair: C. Mark Read, Bechtel Quebec Ltd

9:00 AM Introductory Comments

9:05 AM
Electrode Plant-Larger Anode Assembly Project: *Paul Harry*[1]; [1]McDonald Keen Group Pty Ltd

This project involved converting the existing Electrode facilities from processing the original Sumitomo rod/anode assembly to a new rod/anode assembly. This required replacement of 10,000 rods, (450kg increase per assembly), a changed stub diameter from 150mm to 200mm with new stub geometry, production of a new anode to fit this new stub size and major structural strengthening of the Rodding Room building and power and free conveyors. All Rodding Room processing equipment had to be modified in the correct time sequence to process the new assemblies, and new power and free conveyors and rod load/unload station constructed. The full implementation was done as a rebuild on the run with no operational stoppages. The project had a 10-month time frame from design to completion.

9:30 AM
Anode Stubs Inspection System: *Jean-Pierre Gagne*[1]; Marc-André Thibault[1]; Jean-Yves Carrier[2]; Gilles Dufour[2]; Claude Gauthier[2]; [1]STAS; [2]Alcoa Canada, Aluminerie Deschambault

Anodes consumed in the smelting process for the production of primary aluminium need to be replaced regularly. Cleaning is required on anode butts to remove the waste material. An inspection is necessary to ascertain that the rods need to be repaired before they are fitted with new anodes. STAS is working with Alcoa Deschambault, where until recently such inspection was manually carried out, to develop an automated inspection system. The objectives are to develop and implement a low cost solution to perform the inspection task automatically. The inspection system, based on artificial vision, uses three static cameras and is integrated within the existing conveyor system of the rod plant. Anode rod assemblies are inspected in line while they are transported on the conveyor. This paper presents the initial results obtained with the plant prototype.

9:55 AM
XELIOS™, A Vibrocompactor Designed for Producing High Density Anodes: *Hugues Vincent*[1]; Jean-François André[1]; [1]Solios Carbone

High amperage pot operation requires the use of anodes with high and stable density; this can be a challenge when the quality of coke is degrading. Such anodes can be produced by optimizing the carbon paste process and by applying cover back pressure and vacuum to anode block vibrocompaction. This has been achieved at Smelter A operating at more than 350kA pot amperage with anodes of 1.60 baked density or more. In order to further optimize the vibrocompaction process, a numerical model was developed which predicts the green anode density for a given paste and for given design characteristics of the vibrocompactor. Finally, based on the above results and on a 30 year experience in designing and supplying vibrocompactors to aluminium smelters in the world, a new vibrocompactor, XELIOS™, has been designed to provide optimum performance and cost.

10:20 AM
Understanding Calcined Coke Bulk Density- Inventory: *Bernard Vitchus*[1]; Frank Cannova[1]; [1]BP Coke

Calcined coke inventory accounting is important to both producer and user of calcined coke. The accuracy of calculating the amount of calcined coke in storage is dependent on knowing the volume of calcined coke and its stowage bulk density. Calcined coke stowage bulk density changes due to segregation which changes the size distribution of the coke. Data is presented to show the magnitude of these changes. A more accurate inventory calculation is achieved by adjusting the stowage bulk as a function of calcined coke receipts and silo discharges.

Friction Stir Welding and Processing IV: Session VI

Sponsored by: The Minerals, Metals and Materials Society, TMS Materials Processing and Manufacturing Division, TMS: Shaping and Forming Committee
Program Organizers: Rajiv Mishra, University of Missouri; Murray Mahoney, Rockwell Scientific Company; Thomas Lienert, Los Alamos National Laboratory; Kumar Jata, US Air Force

Thursday AM Room: Northern E3
March 1, 2007 Location: Dolphin Hotel

Session Chair: Kevin Colligan, Concurrent Technologies Corporation

9:00 AM Invited
Stir Zone Temperatures during Friction Stir Processing: *Terry McNelley*[1]; Keiichiro Oh-ishi[2]; Alexander Zhilyaev[3]; Srinivasan Swaminathan[1]; Christian Fuller[4]; Blair London[5]; Murray Mahoney[4]; [1]Naval Postgraduate School; [2]National Institute for Materials Science; [3]Centro Nacional de Investigaciones Metallurgicas; [4]Rockwell Scientific Company; [5]California Polytechnic State University

During friction stir processing the direct measurement of stir zone temperatures, strains and strain rates is difficult due to steep gradients and transients in these quantities. In this work, estimates of local peak temperatures have been made from analysis of stir zone microstructures in a NiAl bronze material and compared to embedded thermocouple and optical pyrometer measurements. Depending on process parameters peak stir zone temperatures of 860–1000°C were estimated from microstructure data and these estimates were confirmed by direct measurements. In addition, strains were estimated from the shape change of microstructure constituents in selected locations in the stir zone.

9:20 AM Invited
Friction Stir Processing of D2 Tool Steel for Enhanced Blade Performance: *Carl Sorensen*[1]; Tracy Nelson[1]; Scott Packer[2]; Charles Allen[3]; [1]Brigham Young Univeristy; [2]Advanced Metal Products; [3]Knives of Alaska

Friction stir processing (FSP) has been applied to blade blanks made from D2 steel to improve blade performance. D2 blanks of moderate hardness (30-40 HRC) are subjected to FSP using a convex scrolled shoulder, step spiral pin (CS4) tool made from PCBN. The resulting microstructures are hard, tough, and corrosion resistant. Hardness on the order 65-68 Rockwell C are achieved consistently. The grain size is on the order of a micron or less. The chromium content remaining in the steel grains is higher than that in quenched and tempered D2. Knife blades manufactured from FSP D2 steel exhibit up to a 10 fold increase in edge life over traditional thermo-mechanically processed and heat treated D2 blades. Methods for repeatably testing blade edge performance are presented, along with a microstructural analysis of the FSP D2.

9:40 AM
The Relationship between Friction Stir Process Parameters and Microstructure of Investment Cast Ti-6Al-4V: *Adam Pilchak*[1]; Z. Tim Li[2]; James Fisher[2]; Mary Juhas[1]; James Williams[1]; [1]Ohio State University; [2]Edison Welding Institute

Titanium alloy castings have a coarse, fully lamellar microstructure which results in lower yield strength and high cycle (HCF) fatigue life than comparable wrought products. A study of FSP has demonstrated the microstructure at the surface can be modified to eliminate the coarse as-cast microstructure. FSP can transform the as-cast microstructure into a range of microstructures, all of which are finer than the as-cast structure. These range from very fine (1 - 2 μm diameter) equiaxed microstructures to lamellar structures with 20-40 μm prior β grains. Such fine-grained equiaxed structures are difficult to produce in wrought products. We have used a variety of characterization techniques to investigate these microstructural changes. The changes will be illustrated and discussed in terms of the FSP parameters. The mechanism for the observed microstructure evolution will be described. This work is supported by the Office of Naval Research under contract N00014-06-1-0089.

9:55 AM
Friction Stir Processing of a Cast WE43 Magnesium Alloy: *Timothy Freeney*[1]; Rajiv Mishra[1]; Glenn Grant[2]; Ravi Verma[3]; [1]University of Missouri; [2]Pacific Northwest National Laboratory; [3]General Motors Research and Development Center

A heat treatable sand cast WE43 magnesium alloy was friction stir processed at 3 increasing heat indices to determine the effects of increasing heat input on mechanical and microstructural properties. In addition, the sequence of solutionizing and aging heat treatment with respect to maximizing the processing efficiency, which is defined as the percent increase of FSP nugget yield strength over base yield strength, was investigated. When no solutionizing was performed after FSP, the processing efficiency was 124%, when a yield strength of 250 MPa was achieved for the cast component in the FSP + T5 heat treatment condition. When compared to the yield strength of 202 MPa in the cast + T6 condition, this increase in mechanical properties is an attractive prospect for the local enhancement of casting properties.

10:10 AM
Determining the Effects of Friction Stir Processing on the Damping Characteristics of Al 5083 and Al/SiC Metal Matrix Composite: *Karl Koch*[1]; Jonathan Lu[1]; Anthony Barajas[1]; William Arbegast[1]; Casey Allen[1]; Abiuda Reddy[1]; [1]South Dakota School of Mines and Technology

Friction stir welding and processing (FSW/P) has been demonstrated to be a reliable and high quality process for joining or microstructural modification a variety of aluminum alloys, even those classified as unweldable by traditional means. For built-up structures fabricated using FSW and subjected to an acoustic vibration environment, there is an opportunity to use novel alloys, joint designs and metal matrix composites (MMC's) to passively manage the vibration response of the structure. A first study has been conducted that investigates the effect of FSW/P on the material damping characteristics. Two tests, a uniaxial cyclic load test and a cantilever beam subjected to forced vibrations, have been use to determine the material damping constants for parent metal and friction stir processed metal in 5083-H111 and an aluminum/SiC MMC.

10:25 AM
Friction Stir Microstructural Modification of Investment Cast F357: *S. Jana*[1]; Rajiv Mishra[1]; H. Chou[2]; Darrell Herling[3]; [1]University of Missouri; [2]The Boeing Company; [3]Pacific Northwest National Laboratory

Cast components offer poor mechanical properties due to its inherent inhomogeneous microstructure. Friction stir processing (FSP) is being developed as a technique to embed wrought microstructure in a cast component and hence improve mechanical properties. A hypoeutectic Al-Si alloy was friction stir processed in this study using various run parameter combination. Tensile test results indicate considerable improvement in properties over the cast component because of refinement in Si particle size. Samples processed at higher tool rotation rate show more uniform and homogeneous microstructure. DSC and TEM were used to establish the precipitation sequence and quantify the size and volume fraction of strengthening phases. Various possibilities for the change in ductility after T6 heat treatment is discussed in context of microstructural changes. This work was performed under the NSF-IUCRC for Friction Stir Processing and the additional support of NSF, GM and Friction Stir Link for the UMR site is acknowledged.

10:40 AM Break

10:55 AM
The Effect of Grain Orientation via FSP on Tensile Behavior: *Ssu- Ta Chen*[1]; Truan- Sheng Lui[1]; Li- Hui Chen[1]; [1]Cheng-Kung University

The structure resulted from FSP is equiaxed recrystallized grain. Nevertheless, the orientation gradient was detected in this study. The tensile behavior was responsible to the texture evolution. Irrespective of the travelling speed, the uniaxial tension applied orthogonal to FSP travelling direction demonstrated good strength than parallel to FSP direction. On the other hand, x-ray diffraction pattern exhibited that the (111)was the main crystallgraphic direction of transverse plane in stirred zone near both advancing side and retreating side, but it was replaced with (220) in the center. The evolution of grains orientation showing meaningful effect to explain the feature of tensile behavior.

11:10 AM
The Effect of Friction Stirring on the Erosion Wear Resistance of Al-Si Alloy: *Tun-Wen Cheng*[1]; Truan-Sheng Lui[1]; Li-Hui Chen[1]; [1]National Cheng-Kung University

The effect of different morphology of Si particles on erosion behavior was investigated in the recent research. Al-Si alloy was selected, and friction stir process (FSP) was used to be a method to change the morphology of Si particles. Ai-7Si alloys have typical ductile erosion behavior although brittle cracking of Si particles coexist with plastic deformation and fracture. Compared to the alloy with acicular Si particles, the alloy with rounded Si particles is superior in erosion resistance.

11:25 AM
Corrosion in Friction Stir Welded Dissimilar Aluminum Alloy Joints of 2024 and 7075: *Christian Widener*[1]; Dwight Burford[1]; Jorge Talia[1]; Bryan Tweedy[1]; [1]Wichita State University

Dissimilar alloy joints are notoriously susceptible to corrosion, especially in 2XXX and 7XXX series alloys. Recently, researchers have shown that this can also be the case in friction stir welded joints; however, an initial temper and post-weld artificial aging combination has been identified which results in remarkably improved exfoliation response when 0.125-inch 2024-T81 is joined to 7075-T73 with 2024-T81 on the advancing side, followed by post-weld artificial aging (PWAA). The improved corrosion response is attributed to the overaged condition of both alloys and the application of a PWAA treatment. Samples were evaluated using optical microscopy, exfoliation, electrical conductivity, microhardness, and tension testing. While it was noted that the 7075-T73 material was preferentially attacked over the 2024-T81 side of the joint, no pitting or selective attack at the dissimilar interface was observed.

11:40 AM
Investigation to Restore the Exfoliation Resistance of Friction Stir Welded Aluminum Alloy 2024: *Christian Widener*[1]; Dwight Burford[1]; Jorge Talia[1]; Bryan Tweedy[1]; [1]Wichita State University

Friction stir welded aluminum alloy 2024-T3, in the as-welded condition, has excellent mechanical properties, good stress corrosion cracking resistance, and damage tolerance comparable to the parent material; however, it is highly susceptible to exfoliation corrosion. Therefore, an investigation into starting temper and post-weld artificial aging (PWAA) was undergone to restore the resistance to exfoliation corrosion without significantly affecting the other material properties. For this investigation, FSW butt-welds were performed in sheets of 0.125" 2024-T3 and 2024-T81 parallel to the rolling direction. The samples were given PWAA treatments for various time and temperature schemes. Thermal treatments were evaluated using optical microscopy, exfoliation, electrical conductivity, microhardness, tensile, and fatigue crack propagation testing. It was found that it was possible to restore the exfoliation resistance to friction stir welded Al 2024 through PWAA to the –T81 temper or when initially welded in the –T81 temper.

11:55 AM Panel Discussion
Moderated by Rajiv Mishra

12:25 PM Concluding Comments

General Abstracts: Electronic, Magnetic, and Photonic Materials Division: Magnetic and Ferroelectric Materials

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Alloy Phases Committee, TMS: Biomaterials Committee, TMS: Chemistry and Physics of Materials Committee, TMS: Electronic Materials Committee, TMS: Electronic Packaging and Interconnection Materials Committee, TMS: Nanomaterials Committee, TMS: Superconducting and Magnetic Materials Committee, TMS: Thin Films and Interfaces Committee
Program Organizers: Long Qing Chen, Pennsylvania State University; Sung Kang, IBM Corporation

Thursday AM Room: Oceanic 7
March 1, 2007 Location: Dolphin Hotel

Session Chairs: Shenyang Hu, Los Alamos National Laboratory; Long-Qing Chen, Pennsylvania State University

9:00 AM
Microstructure Evolution in Giant Magnetostrictive Materials: *Yongmei Jin*[1]; [1]Texas A&M University

Giant magnetostrictive materials exhibit large field induced deformation, which is a result of either intrinsic direct coupling (through magnetostriction) or extrinsic indirect coupling (through magnetocrystalline anisotropy of martensite variant) or both between magnetization and strain. According to the dominant coupling mechanism, giant magnetostrictive materials fall into three types, with Terfenol-D, Ni-Mn-Ga, and Galfenol representative of each type. In all cases, it is the active response of the coupled ferromagnetic and ferroelastic domain microstructure to external magnetic and mechanical stimuli that determines the magnetostrictive properties. A phase field micromagnetic microelastic model is developed to study the microstructure evolution in giant magnetostrictive materials. The model takes into account various coupling mechanisms, automatically describes domain microstructure evolution along kinetically favorable pathways, characterizes giant magnetostrictive materials of different types within a whole picture of magnetostrictive phenomenon, and identifies common and different mechanisms in different materials. Computer simulations based on this model are presented.

9:20 AM
Thin Film Elastic Modulus Measurement by Magnetostrictive Sensor-A Nondestructive Measurement Technique: *Cai Liang*[1]; L.C. Mathison[1]; Bart Prorok[1]; [1]Auburn University

This paper presents the measurement of the elastic modulus of sputter deposited Cr, Cu, Al and SiC thin films with a magnetostrictive sensor. The sensors were actuated to vibrate in their longitudinal resonant mode by employing a modulated A/C field coupled with an external magnetic field bias. The elastic moduli of these films was determined by measuring the sensor's resonant frequency shift relative to the deposited film thickness, 0.25 to 2.0μm. The as deposited films were characterized by XRD and SEM. The measured elastic modulus of Al, Cr and Cr films agreed well with their bulk counterpart values. Detail comparisons of elastic modulus values obtained by different measurement techniques will also be presented. This measurement technique can be cataloged as a nondestructive technique and is well suited and simple enough to provide mechanical property measurements in any film deposition process where the temperature does not exceed 300°C.

9:40 AM
Nanostructured Mn-Al-C Permanent Magnets Produced by Mechanical Milling: Q. Zeng[1]; *Ian Baker*[1]; Z. Yan[2]; [1]Dartmouth College; [2]University of Delaware

Pre-alloyed $Mn5_{0+x-y}Al_{50-x}C_y$ (x = 0-8; y = 0-3) powders were mechanically milled under argon, and the as-milled powders subsequently annealed at temperatures from 350-600°C to produce the ferromagnetic metastable $L1_0$-structured τ phase. Bulk $Mn_{54}Al_{46}$ specimens were annealed under the same conditions for comparison. The effects of the Mn concentration and C additions on phase formation and magnetic properties of the Mn-Al-C alloys were systematically investigated. It was found that the magnetic properties are strongly dependent both on the fraction of the τ phase and its microstructure. There exists a strong influence of the microstructural refinement, due to the ball milling, on the rate of ε phase to τ phase transformation and on the stability of the τ phase. The kinetics of formation and subsequent decomposition of the magnetic τ phase were found to be markedly different in the MM and bulk alloys. Research sponsored by NIST grant 60NANB2D0120.

10:00 AM
High-Gain Magnetic Photonic Assembly Antennas for GHz Frequencies: *Lanlin Zhang*[1]; Gokan Mumcu[1]; Kubilay Sertel[1]; John Volakis[1]; Hendrik Verweij[1]; [1]Ohio State University

Magnetic Photonic Assemblies (MPAs) are expected to have good coupling and significant antenna gain at GHz frequencies. Initial MPA designs, based on finite element simulations, consist of 10-40 unit cells, with each cell composed of two anisotropic di-electric (A) layers and one ferrimagnetic (F) layer. Both layers need to be made as thin sheets, typically 2 × 2 × 0.02" and with low dielectric losses, tan(δ)preferably $<10^{-5}$. Recent investigations have demonstrated that functional A-layers can be made by cutting slices from laminated ceramics with different dielectric constants. The first laminates were made from commercially available ceramics to demonstrate the feasibility of this approach. Homemade laminates prepared from tape-casting and temperature-controlled sintering show good perspectives to realize the tan(δ) $<10^{-5}$ target. Ca-, V-doped $Y_3Fe_5O_{12}$ garnets (CVG) are proposed for the F layers. A citric-gel route is applied for the synthesis of CVG ceramics, taking account its complex composition.

10:20 AM
Evidence of Iron Ion Valence Variation in Ferroelectromagnet $Pb(Fe_{1/2}Nb_{1/2})O_3$: *Ying Yang*[1]; J. M. Liu[2]; H. B. Huang[2]; Z. G. Liu[2]; [1]Nanjing University of Aeronautics and Astronautics; [2]Nanjing University

Lead iron niobate $Pb(Fe_{1/2}Nb_{1/2})O_3$ (PFN) belongs to the series of complex perovskite compounds called ferroelectromagnets. It was considered to be ferroelectrically and antiferromagnetically ordered below a certain temperature and the interaction of the two ordered phase may bring forth many interesting effect. The possible coexistence of ferromagnetism and ferroelectricity may be caused transition element ions which are in the octahedral B(B') positions and can become ordered via an indirect exchange interaction through the oxide ions. The behavior of some characteristic features of $Pb(Fe_{1/2}Nb_{1/2})O_3$ are quite author dependent. Most of the contradictions seem to be related to sample homogeneity. Facing the variety of the earlier reports, we grow single crystals of PFN from high temperature solution growth and concentrate on the study of the single crystal samples or powders obtained by grinding them.

10:40 AM Break

11:00 AM
Nanotwin Diffraction, Adaptive State, and Engineered Domain Configuration in Strongly Piezoelectric Single Crystals: *Yu Wang*[1]; [1]Virginia Tech

We perform diffraction and crystallographic analyses to understand the ultrahigh piezoelectric properties of single crystal $Pb[(Zn_{1/3}Nb_{2/3})_{1-x}Ti_x]O_3$, $Pb[(Mg_{1/3}Nb_{2/3})_{1-x}Ti_x]O_3$. Their superior properties are related to the complicated structural phase transformations involving new intermediate phases near morphotropic phase boundaries, but the origin is yet to be clarified. We develop a nanotwin diffraction theory that predicts an adaptive diffraction phenomenon, where the Bragg reflection peaks are determined by coherent superposition of scattered waves from individual twin-related nanocrystals and adaptively shift along the twin peak splitting vectors according to twin variant volume fraction. It explains the experimentally observed intermediate monoclinic phases and, in particular, the intrinsic lattice parameter relationships. Diffraction and crystallographic analyses describe, in reciprocal space and direct space respectively, the symmetry changes of the engineered domain configurations from nanoscale to macroscopic scale. The analyses attribute the ultrahigh piezoelectric properties to the engineered nanodomain configurations and significant domain size effect at nanoscale.

11:20 AM

Effects of Deposition Conditions on the Dielectric Non-Linearity of Ba0.6Sr0.4TiO3 Thin Films: *Hongwei Chen*[1]; [1]University of Electronic Science and Technology of China

The influences of deposition conditions, such as sputtering power, deposition pressure and sputtering gas, on the microstructures and dielectric non-linearities of barium strontium titanate (Ba0.6Sr0.4TiO3, short for BST) thin films were investigated. The results show that both the dielectric constant and tunability remarkably increase to the maximum when the sputtering power is about 100 W, and then decrease with increasing power. This is attributed to the variation in film thickness as a result of increasing sputtering power. Not only the ratios of (Ba+Sr)/Ti and Ba/Sr but also the root-mean-square (RMS) roughness increases with increasing deposition pressure. The tunability of dielectric constant of BST film increases as O2: Ar ratio increases, which could be attributed to the variations in grain size. At 1 kHz the dielectric constant and the tunability of the BST film with optimum conditions are 1267 and 29.5%, respectively.

11:40 AM

Modeling of Dielectric Nonlinearity of Ferroelectric Ceramics: *Chunlin Fu*[1]; [1]Chongqing University of Science and Technology

In this article, it is assumed that in ferroelectric ceramics there only exist cubic-shaped grains with grain size, which are all uniform, in order and surrounded by grain boundaries with width. Moreover, it is assumed that the dielectric nonlinearity of ferroelectric ceramics is only contributed by the grains. And then the grains and the grain boundaries were modeled in terms of capacitors and resistors. After a series of mathematic derivations, the functions of C-V and P-E were obtained. Based on our model for dielectric nonlinearity of ferroelectric crystals [J. Appl. Phys., 2005, 97(3): 034110], a model, including the grain size and the grain boundary width, for dielectric nonlinearity of ferroelectric ceramics was established. The accuracy of the model prediction was quantitatively verified by our experimental data. The results proved that the above model can describe the dielectric nonlinearity of ferroelectric ceramics.

12:00 PM

Effect of Annealing on Depletion Layer Width and Schottky Barrier Height of Pt/$Ba_{0.6}Sr_{0.4}TiO_3$ Interface: *Chunlin Fu*[1]; Wei Cai[1]; Fusheng Pan[1]; [1]Chongqing University of Science and Technology

$Ba_{0.6}Sr_{0.4}TiO_3$ thin films were prepared by rf-magnetron sputtering system. The effect of annealing on depletion layer width and Schottky barrier height of Pt/BST interface is investigated. The results show that the depletion layer width of the as-deposited BST film is about 3~5 times greater than that of the annealed film. For as-deposited samples, the Schottky barrier height increases with increasing temperature and voltage, and the effective Richardson constant almost linearly increases as the square of voltage increases. However, for annealed samples, the Schottky barrier height linearly decreases with increasing voltage and is almost independent upon temperature, and the effective Richardson constant almost linearly decreases with the increasing square of voltage.

12:20 PM

Formation of Nanocrystalline Structure in Metals by Severe Plastic Deformation: *Yoshikazu Todaka*[1]; M. Umemoto[1]; J. Li[1]; A. Yamazaki[1]; C. Wang[1]; J. Sasaki[1]; K. Tsuchiya[1]; [1]Toyohashi University of Technology

In the last few decades, severe plastic deformation (SPD) technique has been applied widely to design ultrafine-grained materials, especially nanocrystalline (NC, grain size smaller than 100 nm) materials, withimproved properties due to its simplicity and applicability for all class of materials. Submicron-grained materials can be successfully produced by most SPD processes. However, NC structure can not be formed by heavy cold-rolling, equal channel-angular pressing (ECAP) or accumulative roll bonding (ARB) which are homogeneous deformations with large amounts of strain (equivalent strain > 5). While, NC materials are obtained by non-homogeneous deformation processes with large strain gradients, such as high-pressure torsion (HPT) deformation, ball milling, shot peening and drilling. J.G. Sevillano explained that high density of geometrically necessary dislocations is generated by applying large strain gradient and these dislocations contribute to the formation of NC structure and to the extra strengthening.[1] In the present study, HPT deformation was carried out to understand the conditions necessary to obtain NC structure in various metals. The maximum hardness (Hv 5 GPa) in the Fe - 0.03 mass% C disk after HPT-straining was twice higher than the hardness (2.4 GPa) obtained by heavy cold-rolling. At the center of HPT-processed disk, where shear strain is nominally zero, the hardness increased up to the saturation value of 3.3 GPa. These results show that strain gradient contributes to strengthening and to grain refinement. However, the grain refinement was saturated with around 200 nm in layered grain thickness although the HPT-processed disk was applied large strain and strain gradient. This suggests that not only strain gradient and strain but also other deformation conditions are necessary to form NC structure. The other necessary conditions to form NC structure by deformation are discussed. [1]J.G. Sevillano: Proc. of 25th Riso Int. Symp. on Mater. Sci., ed. by C. Gundlach et al., Denmark, (2004), 1.

General Abstracts: Electronic, Magnetic, and Photonic Materials Division: ZnO Thin Films and Liquid Crystals

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Alloy Phases Committee, TMS: Biomaterials Committee, TMS: Chemistry and Physics of Materials Committee, TMS: Electronic Materials Committee, TMS: Electronic Packaging and Interconnection Materials Committee, TMS: Nanomaterials Committee, TMS: Superconducting and Magnetic Materials Committee, TMS: Thin Films and Interfaces Committee
Program Organizers: Long Qing Chen, Pennsylvania State University; Sung Kang, IBM Corporation

Thursday AM
March 1, 2007
Room: Oceanic 4
Location: Dolphin Hotel

Session Chairs: Yongmei Jin, Texas A&M University; Sung Kang, IBM T.J. Watson Research Center

9:00 AM

Investigation of Carrier Type Conversion of Post Annealed ZnO:P Thin Films as a Function of the Substrate Temperature: *Hyunsik Kim*[1]; Jean Erie[1]; Stephen Pearton[1]; David Norton[1]; Jau-Jiun Chen[2]; Fan Ren[2]; [1]Department of Materials Science and Engineering, University of Florida; [2]Department of Chemical Engineering, University of Florida

The transport properties of phosphorus-doped ZnO films were investigated as a function of the substrate temperature. The ZnO:P films were grown on sapphire (0001) substrates by pulsed laser deposition with different substrate temperature in the range of 600~800°C and post thermal annealing was performed at 850~ 950°C under oxygen ambient. As-grown ZnO:P samples showed n-type characteristics with 10^{16} ~ 10^{17} /cm^3 electron concentration regardless of the growth temperature. However, after the thermal annealing, the samples grown at 700 and 750°C converted to p-type having a hole concentration of 10^{16} ~ 10^{17} /cm^3, a mobility of 0.3 ~ 0.7 cm^2/ V-s, and a resistivity of 17~21 Ω-cm, while the samples grown at other temperatures still remain as n-type even after thermal annealing process. The properties of these films will be described. This research was sponsored by the Department of Energy (grant DE-FC26-04NT42271).

9:20 AM

The Effects of Nitrogen Doping on Structural and Electrical Properties of ZnO Thin Films: *Makoto Hirai*[1]; Ashok Kumar[1]; [1]University of South Florida

Zinc oxide (ZnO) thin films have been synthesized by irradiating laser light on ZnO plate in high vacuum and nitrogen (N2) ambient pressure. The homostructural devices, which consisted of undoped ZnO and N doped ZnO thin films, indicated the current-voltage curves attributed to the formation of p-n junction. This fact can be stated that the N doped ZnO thin films have p-type conductivity. Additionally, in the N doped ZnO thin films, utilizing x-ray diffractometer and ultraviolet-visible spectrometer, the decrease of interplanar spacing and the shrinkage of band gap occurred with increase in the N2 ambient pressure. The interplanar spacing seems to reduce that the length of Zn-N bond is shorter than that of Zn-O bond. The band-gap narrowing may be due to the difference in the electronegativity of nitrogen and oxygen. Moreover, this investigation will be also discussed the change in internal stress induced by the incorporation of N atoms.

9:40 AM

Optical and Structural Properties of ZnO Thin Films Grown by Metalorganic Chemical Vapor Deposition: *William Fenwick*[1]; Tahir Zaidi[1]; Nola Li[1]; Shalini Gupta[1]; Zhe Feng[2]; Ian Ferguson[1]; [1]Georgia Institute of Technology; [2]Graduate Institute of Electro-Optical Engineering, National Taiwan University

We have successfully built a Metalorganic Chemical Vapor Deposition system for the growth of ZnO materials. This paper investigates their optical and structural properties by way of high resolution X-ray diffraction (HR-XRD), photoluminescence (PL), Raman scattering (RS), and other techniques such as atomic force microscopy, UV-Visible optical transmission, and reflectance. Room temperature PL measurements show a bandedge emission peak near 3.28 eV, and in some samples, a green defect band at about 2.4 eV, suggesting oxygen-related defects. Raman measurements show the E2(high) and A1(LO), and sometimes the A1(TO) and other defect bands. HR-XRD measurements show a variation of the (0002) peak linewidth between 170 - 400 arcsec, depending on growth conditions such as VI/II ratio, growth pressure, growth temperature, precursor injection pressure, disk rotation speed, and total volume flow. Interesting variations from other measurements are also observed, revealing the growth physics and chemistry related to the ZnO materials studied.

10:00 AM

Magnetic and Structural Properties of Fe Doped ZnO Thin Films: *Soo-young Seo*[1]; Sun-hong Park[1]; Chang-ha Kwak[1]; Yong-byung Lee[1]; Seon-hyo Kim[1]; [1]Pohang University of Science and Technology

A Fe doped ZnO thin films were grown on a a-sapphire substrate by RF magnetron sputtering. The structures of the Zn1-xFexO films with the composition ratio of Fe were studied with Fe-SEM, XRD, AFM and EXAFS. The XRD measurements showed Zn1-xFexO films with x=0.03, 0.05, 0.07 have a wurtzite structure like ZnO crystals without any extra phase. However, the (0002) diffraction peak moved from 2Θ=34.42° to 34.1° as x is increased. This implied the lattice constant c was increased by about 0.047Å due to Fe replacement on the Zn site. The structural environments around Zn atoms in the thin films were studied with XAFS. XPS measurements were employed to characterize the valence state of Fe ions. From the XPS data, we can rule out the existence of Fe metal clusters. In addition, we introduce Superconducting Quantum Interference Device measurement in order to determine the magnetic properties of Zn1-xFexO thin films.

10:20 AM Break

10:40 AM

Dimension Optimum Phenomenal magnonequation For Nematic Liquid Crystal: *Chia Fu Chang*[1]; Zou-ni Wan[1]; Chia-Hi Chen[1]; [1]Kun Shan University of Technology

The transition can be approached by changing the impurity concentration or, indirectly, by tuning the temperature since the pinning strengths of the random and crystal potential have in general a different temperature dependence. The nematic liquid crystal is clear only when a long range order exists, in the whole medium using the Jones matrix method. Director can change from point to point and is, in general, a function of space. These two technologies have ca used more and more product designers to turn to liquid crystal (LC) displays, which have consequently experienced phenomenal growth. The resist profile simulation is carried out using the combined data thus obtained. Details of the lens structure and of the devices fabrication and performance are described. Light from conventional light source or laser is passed through a polarizer and then incident on the specimen. Liquid crystal displays has fostered continued development, to the point where full color video displays have been realized which can rival. At the nematic isotropic, transition temperature, the medium becomes isotropic and looks clear and transparent.

11:00 AM

Quasielastic Phenomenological Isotropic Optimization Medium Simulation for Phenomenal Liquid Crystal: *Chia Fu Chang*[1]; Wi-Ci Chen[1]; Zou-ni Win[1]; [1]Kun Shan University of Technology

The problems of these two technologies have caused more and more product designers to turn to liquid crystal (LC) displays, which have consequently experienced phenomenal growth. The success of liquid crystal displays has fostered continued development, to the point where full-color video displays have been realized which can rival. Details of the lens structure and of the devices fabrication and performance are described. Simulation using the Jones matrix method. Direction can change from point to point and is, in general, a function of space. The transition can be approached by changing the impurity concentration or, indirectly, by tuning the temperature since the pinning strengths of the random and crystal potential have in general a different temperature dependence. Light from conventional light source or laser is passed through a polarizer and then incident on the specimen. The resist profile simulation is carried out using the combined data thus obtained. The nematic liquid crystal is clear only when a long range order exists, in the whole medium. At the nematic-isotropic, transition temperature, the medium becomes isotropic and looks clear and transparent.

11:20 AM

Preparation and Characterization of Cu-Coated Graphite by Electroless Copper Plating: *Liu Wei*[1]; Yao Guangchun[1]; Liu Yihan[1]; [1]Northeastern University

In order to solve the wettability quantity of graphite/copper interface and improve the capability of Copper–graphite composite materials, the Cu-coated graphite was prepared by redox reaction that zinc as reducing agents and blue vitriod as oxidizing agents. This paper studied the factors that affected the plating film. Under the optimizing process without additions the Cu-coated graphite assumed brassy color and the plating films united tightly with graphite examined with scanning electron microscopy. The experiment proved that this kind of electroless copper plating has advantage of steadily electrolyte, plating speedy and high quality of plating films.

11:40 AM

Electrochemistry of the Electro-Deoxidation of Silicon Dioxide in CaCl2 and NaCl Melt: *Shulan Wang*[1]; [1]Northeastern University

The electro-deoxidation of silicon dioxide in equalmolar CaCl2 and NaCl was studied by electrochemical measurements. Three cathodic current peaks in the cyclic voltammogram and three response semicircles in the A.C impedance spectra were observed and are concerned to the electro-deoxidation reaction of SiO2. Intermediates SiO, SiO, CaSiO3 and Ca2SiO4 were detected by XRD and support the following reaction mechanism: 2SiO2 + CaO + 2e- = SiO + CaSiO3+ O2- CaSiO3+ SiO+CaO+2e- =Si + Ca2SiO4 +O2- Ca2SiO4 + 4e- = Si + 2CaO +2O2- The charge transfer resistances and the activation energies were obtained by simulating the AC impedance spectra with equivalent circuits. The electro-deoxidation reaction of SiO2 was controlled by the diffusion step, Free oxygen ions were released and CaO is the catalyst of the process.

General Abstracts: Materials Processing and Manufacturing Division: Processing and Microstructural Development

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 Modeling Analysis and Control Committee, TMS: Shaping and Forming Committee, TMS: Solidification Committee, TMS: Surface Engineering Committee

Program Organizers: Fernand Marquis, Naval Postgraduate School; Ralph Napolitano, Iowa State University; Neville Moody, Sandia National Laboratories

Thursday AM — Room: Northern A2
March 1, 2007 — Location: Dolphin Hotel

Session Chair: Henry Young, Wright State University

9:00 AM

Extrusion of a Solvated Polymer into a Moving Viscous Medium Allows Generation of 300nm Polymer Fibers via Hydrodynamic Focusing: *Henry Young*[1]; Murali Gorantla[1]; Sonya Boone[1]; Chad Clark[1]; Mostafa El-Ashry[1]; [1]Wright State University

We present a wet fiber spinning technique that involves injection of a solvated polymer into a highly viscous moving medium through a micro-aperture. Fibers as small as 300 nm have been observed. Video microscopy

is used to characterize this process, and significant fiber diameter reduction is observed to occur in close proximity to the point of precursor injection. Hydrodynamic focusing, in which a flow mismatch between the precursor and surrounding media causes fiber draw-down, is hypothesized to control this effect. This may be the dominant draw-down mechanism in a process that can produce truly continuous nanofiber. This method is capable of generating fibers from precursors with viscosities that would render them unspinnable by any other known method.

9:25 AM

Alumina-Aluminum Titanate-Titania Nanocomposite Coating on 316L Stainless Steel for Biomedical Applications: *Leonardo Rocha*[1]; Samar Kalita[1]; [1]University of Central Florida

Recent years have seen efforts in developing nanostructured bioceramics for bone therapeutic. The ability to apply bioceramics as strong adherent coating on bio-metals is critical. While many bioceramics are being used as coatings, alumina-aluminum titanate-titania (Al_2O_3-Al_2TiO_5-TiO_2) nanocomposite has yet to find its niche. This research produced stable Al_2O_3-Al_2TiO_5-TiO_2 nanocomposite coatings using sol-gel processing and spin-coating. Aluminum isopropoxide and titanium isopropoxide were used as precursors. N-proponal was used as solvent. The two sols obtained were mixed under vigorous stirring, maintaining sol pH at 5.5. The resultant was refluxed at 120°C for 2 h, producing a gel. This gel was used to spin-coat 316L substrate at varying times, 12, 15 and 20 sec, and at 3000 RPM. The acceleration speed of 980 RPM, with time of 5-8 sec was used for uniform gel spreading. The final coatings were characterized using SEM, XRD and Pull-Out tests. *In vitro* bioactivity was accesses in SBF.

9:50 AM

Complex Biocompatible Nitinol Structures Enabled by Reactive Eutectic Brazing with Niobium: *J. W. Foltz*[1]; K. B. Low[1]; J. A. Shaw[2]; D. S. Grummon[1]; [1]Michigan State University; [2]University of Michigan

We have recently developed a brazing technique for NiTi based on the quasi-binary TiNi-Nb eutectic system. At 1170°C, contact between TiNi and Nb produces a liquid with a composition near 36Ti-36Ni-28Nb that aggressively wets mating surfaces without fluxes. The solidified braze microstructure is strong and ductile, as evident by tensile data and fracture surfaces. The process may be used with both shape memory and superelastic alloys, as well as porous nitinol and NiTi thin films. Tensile data shows that the full thermoelastic transformational functionality of the base material can be retained with proper post-braze heat treatment. Sputtered NiTiNb multilayers of eutectic composition may be used as the braze alloy to minimize attack of base material by the reactive liquid. We show how complex built-up structures, such as honeycombs and spaceframes, can be fabricated, and that the approach can be extended to the joining of NiTi to other biomedical alloys.

10:15 AM

Microstructural Development during Gas Tungsten Arc Welding (GTAW) of Silicon and Aluminum Based Transformation Induced Plasticity (TRIP) Steels: *Murugaiyan Amirthalingam*[1]; Marcel Hermans[2]; Ian Richardson[3]; [1]Netherlands Institute for Metals Research; [2]Delft University of Technology; [3]Netherlands Institute for Metals Research/Delft University of Technology

In this work, microstructrual development in Gas Tungsten Arc welded (GTAW) silicon and aluminum based TRIP steels was studied by optical and electron microscopy. X-ray diffraction measurements were carried out to estimate the retained austenite contents in the heat affected and weld zone microstructures. The fusion zone of both welds contained complex inclusions. Energy Dispersive Spectroscopic analysis on these inclusions showed that the centre of the inclusions contained oxides of silicon and aluminium in silicon and aluminum based steels respectively. Epitaxial enrichment of manganese, sulphur and phosphorous was found on the oxides in the inclusions. The fusion line of aluminium based steel weldments contained higher amounts of allotriomorphic ferrite than silicon based steel weldments due the segregation of aluminium in the fusion line during solidification. Very small amounts (about 2%) of retained austenite were found in the fusion zones as compared with the base metal which contain about 10%.

10:40 AM

Effect of CeO2 on the Preparation and Properties of Nickel-Plated Carbon Fiber Reinforced 2024 Alloy Matrix Composites: Tianjiao Luo[1]; *Guangchun Yao*[1]; Linli Wu[1]; Yihan Liu[1]; [1]Northeastern University

The rare earth oxide CeO2 was investigated as the addition agent for the preparation of 2024 alloy matrix composites reinforced with Ni-coated carbon fibers, and the effect of CeO2 on the dispersity of carbon fiber, porosity and mechanical properties of the 2024 alloy matrix composites reinforced with Ni-coated carbon fibers was researched in this paper. The behavior of CeO2 in the aluminum alloy matrix composites reinforced with Ni-coated carbon fibers was discussed according to the fluid mechanics principle, the material processing principle and the results tested by using the advanced analytical method, such as Scanning Electron Microscopy (SEM) and tensile test. The analysis shows that CeO2 can make the dispersion of carbon fiber even in the composites, and can reduce the porosity of composites, and can increase the tensile strength by 23% and the yield strength by 26% of the rolled composites.

11:05 AM

Controlling Aspect Ratio of Aragonite Precipitated Calcium Carbonate at Low Temperature: *Woon Kyoung Park*[1]; Ji Whan Ahn[1]; Choon Han[2]; [1]Korea Institute of Geoscience and Mineral Resources; [2]KwangWoon University

It was synthesized metastable phase aragonite precipitated calcium carbonate at high temperature. Aragonite precipitated calcium carbonate with high aspect ratio was synthesized at high reaction temperature and concentration of Ca(OH)2 slurry. In this research, it was synthesized homogeneous aragonite precipitated calcium carbonate used to additives on reaction with Ca(OH)2 and CO2 gas at room temperature. It used MgCl2 as additives. To control aspect ratio of aragonite precipitated calcium carbonate used aragonite seed at low temperature with aspect ratio 5. In this result, aragonite precipitated calcium carbonate increased at aspect ratio over 20.

11:30 AM

The Investigation on Bio-Oxidation of Arsenopyrite: *Li Qian*[1]; [1]Central South University

An investigation on oxidation of arsenopyrite with thiobacillus ferrooxidans in 9k solution was conducted. The results showed that addition proper quantities of FeS2 or Fe3+ would promote As3+ oxidized to As5+, and increase the activity of the bacteria during the bio-oxidation of arsenopyrite. Under low pH, microbes are hard to live, and if the pH is higher, there will be deposition ([KFe3(SO4)2(OH)6]),which inhibits the oxidation process. The sizes of sample particle should be in a reasonable range. When the sizes are under 0.074mm, the oxidation rate is ideal. In the range of temperature, low temperature is suitable for thiobacillus ferrooxidans growth. When the rotating speed is too high or too low, the oxidation rate is low.

General Abstracts: Materials Processing and Manufacturing Division: Structure/Processing/ Properties Relationships

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 Modeling Analysis and Control Committee, TMS: Shaping and Forming Committee, TMS: Solidification Committee, TMS: Surface Engineering Committee

Program Organizers: Fernand Marquis, Naval Postgraduate School; Ralph Napolitano, Iowa State University; Neville Moody, Sandia National Laboratories

Thursday AM — Room: Northern A1
March 1, 2007 — Location: Dolphin Hotel

Session Chair: Chris Crosby, Life Cycle Engineering

9:00 AM

Reliable and Accurate High-Performance Infrared Sensors for Aluminium and Non-Ferrous Metals Processing: Francois Reizine[1]; *Frank Conte*[1]; [1]American Sensors Corporation

Infrared sensors for temperature detection, positioning of edges, centering, width control, crop shear optimization, etc. The sensors are accurate even in the presence of steam, water, mist, and can be used for all metals with any roughness, for emissivity as low as 0.1, and temperature of less than 200 C.

The new sensors are digital, so they can easily communicate with the PLC when the product material changes. The reliability and accuracy is maintained for all products and all temperatures. These sensors are important for those who wish to improve quality, reduce down time, reduce maintenance, and increase productivity.

9:25 AM

Reliability Excellence: A Case Study of Success for Commodity-Based Industry: *Paul Campbell*[1]; [1]Alcoa Inc.

The aluminum industry today is faced with external forces that put pressure on companies to achieve financial goals, deliver unparalleled customer service, satisfy safety and regulatory compliance, and fully leverage existing resources in terms of both capital assets and the workforce. Organizations are challenged with reducing costs, increasing revenue, improving profitability, and digging deeper to harness additional capacity. Like most process/discrete manufacturers, the aluminum industry today operates with a "be good, or be gone" mantra. In this presentation learn how a top performing organization, Alumax Mt. Holly, focused on reliability and the role of Operations in asset reliability, and achieved measurable outstanding results through the application of culture, principles, and work processes/technologies – further differentiating itself from the competition. This facility, now owned by Alcoa, implemented LCE's Reliability Excellence methodology throughout their plant portfolio worldwide, assuring Alcoa's sustainability in a fierce global economy, now and well into the future.

9:50 AM

Rapid Assessment of Surface Treatment Effectiveness and Degradation by Direct Field Measurement: *Curtis Rideout*[1]; Scott Ritchie[1]; [1]Positron Systems, Inc.

The generation of compressive residual stresses both on surfaces (e.g., shot peening) and in fastener holes (i.e., cold expansion) are methods for enhancing the fatigue life of components in aircraft structures by retarding crack initiation and growth. Accurate measurement of induced or operational residual stress/strain with current methods is difficult because of the presence of textured materials such as wrought aluminum or the inability to detect damage more than a few microns into a cold worked surface. Positron Systems' Induced Positron Analysis (IPA) can quantify small changes in microstructure induced by surface treatments. The IPA technology provides early indications of impending failure or degradation of treated components and can be used in the assessment of the relative effectiveness of competing surface coating/treatment technologies. Case histories such as the analysis of shot peening treatments/near surface residual stress in variety of materials, coating assessments and heat treatment assessments will be discussed.

10:15 AM

Damage and Performance Property Evaluations of Modified Asphalts Produced by a Novel Modification Technology: *Hossein Ajideh*[1]; Bryan Burris[2]; Hussain Bahia[3]; James Earthman[4]; [1]University of California, Irvine; [2]Petrochem Manufacturing, Inc.; [3]University of Wisconsin-Madison ; [4]Henry Samueli School of Engineering, University of California

There is an increasing interest in using modified asphalts to address deterioration of roads due to severe climate and traffic conditions. One of the oldest asphalt modification techniques is oxidation without additives to change the molecular structure. The present study is designed to investigate rheological, damage and performance related properties of Binary Modified Asphalts (BMAs) and, in particular, a specific oxidization technology with/without polymers designed to improve rutting (creep) resistance, fatigue behavior, and moisture damage properties of the selected binders. The present research revealed an improvement in binder rutting, fatigue, aging, and moisture damage resistance of typical mixtures for BMA. This work also includes a study of the factors affecting the oxidation and rutting at increased stress levels. The results demonstrate the promise of combining the present oxidation technique with polymer additions to optimize performance.

11:05 AM

Surface Modification through CBN Cutting Tool in High Speed Machining: *Venkata Mandava*[1]; G. Janardhan[1]; Ramesh Nunna[2]; [1]Jawaharlal Nehru Technological University; [2]Vallurupalli Nageswara Rao Vignana Jyothi Institute of Engineering and Technology

A significant observation in High Speed Machining is the use of a suitable cutting tool. Diffusion of cutting tool material in to the machined surface is unavoidable during such high speed machining. In this work it is decided to study the effect of percentage diffusion on the properties of machined surfaces. CBN cutting tool is used to the two different materials viz. Al alloy and hardened steel. The various parameters selected are speed, feed and depth of cut, by Energy Dispersive X-Ray Analysis. The experiments are conducted based on DOE.

10:40 AM

Effect of Pre, Post Heat Treatment and also Wire on Mechanical Properties of AISI4130 Steels Welded by TIG Process: *Ali Emamian*[1]; [1]TWI

Because of advantage of 4130 and its group (Cr and Mo) alloys we decided to define a project for aircraft industries. Select test coupon which same material with 2 type of wire 1-Same composition with parent metal 2- low carbon and high alloy with 3 treatment condition 1- without any treatment 2-with only preheat 3-with preheat and post heat condition implement in test coupons each test coupon has tensile strength , guided bend , and impact and metallographic samples. All in all we could conclude the best condition for welding of this type and range of steels . With investigation of structure of HAZ and weld lines we could assess that for best mechanical properties we must control the micro structures. The best condition was for low carbon low alloy with pre and post heat treatment.

11:30 AM

Performance Characteristics of Superalloy Materials for High Temperature Resistance to the Hot Zone Components of Gas Turbine with F-Technology: *Ramarao Adapa*[1]; N. D. Reddy[2]; V. K. Sharma[3]; [1]GRIET; [2]Osmania University; [3]Jawaharlal Nehru Technological University

The effects of Superalloy materials with Nickel and Cobalt based for High temperature resistance, High corrosion resistance and Good Creep behavior in Gas Turbine, has been investigated, to establish the enhanced Power Output and Thermal Efficiency in the filed of Power generation by Gas Turbines (GT). With the F-Technology method the Fire point is advanced to get the high increase of Turbines Inlet Temperature (TIT) which in turns to get enhanced Power Output as well as Thermal Efficiency. The materials like Ni Cr Mo V, Hastally-X and Inconel with Nickel based the performance results are analyzed for continuous high temperature services without any troubles. These materials also studied their machinability and longer life. With the application of these advanced materials, the enhanced performance results are recorded and presented with the practical results. Ni Cd Electro coating and Plasma coating on these selected materials preferred and investigated.

11:55 AM

Challenges in Materials Processing: Role of Heterogeneity in Chemistry and Structure: *C. Sudha*[1]; [1]Indira Gandhi Centre for Atomic Research, Kalpakkam

Challenges in the processing of materials arising due to restructuring of microchemistry and microstructure during service life, are illustrated with the following examples: *Prediction and experimental confirmation of formation and prevention of hard brittle zone in dissimilar joints of ferritic steels. *Optimizing the formation of dilution layer in Colmonoy weld overlay on AISI 304 (L) stainless steel. *Prediction and confirmation of alternate structural material for electrodes of elementary neutral particle detectors. *"Self wastage" of 9Cr-1Mo steel in Sodium water reaction testing facility. In all the above examples, it is demonstrated that detailed computations along with selected confirmatory experiments are essential to recommend appropriate process parameters and also to ensure satisfactory performance of materials.

General Abstracts: Structural Materials Division: Processing and Properties of Light Metals

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Alloy Phases Committee, TMS: Biomaterials Committee, TMS: Chemistry and Physics of Materials Committee, TMS/ASM: Composite Materials Committee, TMS/ASM: Corrosion and Environmental Effects Committee, TMS: High Temperature Alloys Committee, TMS/ASM: Mechanical Behavior of Materials Committee, TMS/ASM: Nuclear Materials Committee, TMS: Product Metallurgy and Applications Committee, TMS: Refractory Metals Committee, TMS: Superconducting and Magnetic Materials Committee, TMS: Titanium Committee
Program Organizers: Rollie Dutton, US Air Force; Ellen Cerreta, Los Alamos National Laboratory

Thursday AM Room: Europe 6
March 1, 2007 Location: Dolphin Hotel

Session Chair: Jay Tiley, Air Force Research Laboratory

9:00 AM Introductory Comments

9:10 AM
New Techniques for Detecting Early Fatigue Damage Accumulation in Aircraft Structural Components: *Curtis Rideout*[1]; David White[1]; [1]Positron Systems, Inc.

The remaining safe operational life of flight critical aircraft structural components prior to crack initiation and detection is currently estimated by fatigue and fracture models supplemented by destructive testing. To provide an acceptable margin of safety, analytical and test results are typically reduced by a factor of from two to four. Induced Positron Analysis (IPA) was investigated and evaluated to determine IPA's capability to measure operationally induced fatigue damage accumulation in thick and multilayer aircraft structural components. For example, F-16 wing attach fittings (WAFs) made of 7475-T3751 aluminum with operational histories that varied from "as manufactured" through "end of life" were obtained and evaluated using IPA. Results of the WAF damage measurements demonstrated the potential for IPA to quantify fatigue damage accumulation, correlate damage accumulation with operational usage, and enhance life prediction models. This paper will discuss the IPA technology, its applications, and the results of the WAF investigation.

9:30 AM
The Role of Interstitials on the Dynamics of Deformation Twinning: Paul Oberson[1]; *Sreeramamurthy Ankem*[1]; [1]University of Maryland

Traditionally it is believed that deformation twins grow at very high speeds, approaching that of the speed of sound. However, recent investigations show that the twins can grow at speeds many orders of magnitude less than the speed of sound during room-temperature creep of alpha (HCP) and beta (BCC) titanium alloys. This origin for this phenomenon appears to be related to the non-conservation of interstitial sites at the twin-matrix interfaces. The extent of non-conservation depends on the crystal structure and the type of twins. Therefore, if interstitial elements are present in the materials, they can affect the rate of twin growth. In this investigation, these developments are reviewed and the ramifications of these findings will be presented. This work is being supported by the National Science Foundation under grant number DMR-0513751.

9:50 AM
Fatigue Crack Initiation in an α + β Titanium Alloy at Ultrasonic Frequencies: *Christopher Szczepanski*[1]; J. Jones[1]; [1]University of Michigan

The role of microstructural variability on the very long life fatigue behavior of a Ti-6Al-2Sn-4Zr-6Mo α + transformed β alloy has been investigated. Ultrasonic fatigue techniques have been used to examine lifetimes as long as 109 cycles. Fatigue crack initiation and early propagation is associated with primary alpha (αp) facets. The size and spatial distribution of ap has been quantified and crack initiation does not appear to depend on these factors. An analysis of crystallographic orientation of the ap facets in the crack initiation regions has been conducted by performing OIM of serial sections. The role of crystallographic orientation of primary alpha on crack initiation and early crack growth will be described.

10:10 AM
Effect of Joint Strength on the Compressive Properties of Periodic Cellular Metals Fabricated by Resistance Brazing: *Eral Bele*[1]; Glenn Hibbard[1]; [1]University of Toronto

Periodic cellular metals (PCM) are an attractive choice in instances where strong light-weight structures with multifunctional capabilities are desired. This investigation addresses a previously unstudied method of their fabrication: joining perforated and deformed aluminum sheets by resistance brazing. The effect of joint strength on the compressive performance of PCM sandwich structures is examined. It is found that resistance brazing can be used to successfully fabricate PCM sandwiches rapidly and inexpensively. Furthermore, it is shown that the resistance brazed joints can readily be made strong enough such that failure occurs in the parent material and the structural capacity of the periodic cellular architecture is not diminished.

10:30 AM
Tribological Performance of Boronized Ti6Al4V Alloy against Si3N4 Ball: *Erdem Atar*[1]; Huseyin Cimenoglu[1]; Eyup Kayali[2]; [1]Gebze Institute of Technology; [2]Istanbul Technical University

In this study, the wear performance of boronized Ti6Al4V alloy has been examined. Boronizing has been carried out in commercial Ekabor II boriding powder at 1100°c for 2.5 h. Characterization of the boronized surface was made by microscopic examinations, hardness measurements and X-ray diffraction analysis. Wear tests were performed under dry sliding and lubricated conditions at room temperature on a reciprocating wear tester by rubbing Si3N4 balls. Boronizing resulted in formation of uniform and compact layer having thickness of about 10 µm on the surfaces of the samples. The surface hardness of the samples was increased from 350 to 2700 HV upon boronizing. XRD studies revealed that surface layer was composed of TiB and TiB2 phases. When compared to the untreated alloy, the wear rate of boronized Ti6Al4V alloys was almost negligible. Under both testing conditions (dry sliding and lubricated) boronised alloy exhibited lower friction coefficient than untreated alloy

10:50 AM Break

11:10 AM
Wear Behaviour of Aluminum Matrix Composites in Water: *Eyup Kayali*[1]; Harun Mindivan[1]; Huseyin Cimenoglu[1]; [1]Istanbul Technical University

In this study, wear behaviors of aluminum alloy matrix 50 vol. % SiC particulate reinforced composites were investigated. Composites were produced by squeeze casting technique by utilizing 2618, 7012 and 7075 aluminum alloys as the matrix and abrasive grade green 30 ìm SiC particles as the reinforcement. Wear tests were conducted in dry air and in water by rubbing Al2O3 balls on the surfaces of composites on a reciprocating wear tester. Wear tests were carried out at the mean contact pressure of 0.6 GPa in dry air conditions and at 2.4 GPa in water. The results of the wear tests revealed that, in dry air sliding conditions, where wear progresses by removal of SiCp's from contact surface, wear resistance is strongly related to the hardness. Even if the mean contact pressure is four fold higher than in dry air sliding wear, SiCp's remain on the contact surface and composites exhibit considerably high wearresistance and noticeably low fiction coefficient in water.

11:30 AM
Structural Behavior and Pressure Cycling Effect Studies of Li-Based Complex Hydrides: *Wen-Ming Chien*[1]; Joshua Lamb[1]; Dhanesh Chandra[1]; [1]University of Nevada - Reno

The effects of pressure cycling are important for long-term reliability of Li-based hydrides during loading/releasing hydrogen. To study the degradation of hydrogen storage capacities, the industrial grade hydrogen contained with low level impurities (O2, H2O, CO/CO2) was used for this hydriding/de-hydriding cycling studies. Equilibrium isotherms were obtained by Sievert's apparatus after 1, 56, 163, and 1100 pressure cycles on imide/amide system, and observe hydrogen capacity changes as a function of cycles at 255oC. Pressure cycling results showed 2.55 (~10.25 bar) and 2.95 wt% (~0.86 bar) hydrogen storage loss after 1100 cycles. Structural studies of the products (desorbed condition) after pressure cycling showed mainly Li2NH and LiH phases, and the impurity Li2O phase. Qualitative X-ray diffraction results showed the Li2NH

reduced from 77% to 13%, and LiH phase increases from 18% to 57% after 1100 cycles. Detail results of structural behaviors and pressure isothermals of different cycles will present.

11:50 AM

Study on Preparation Technique of Pure Al Matrix Foam: Li Bing[1]; Yao Guang-Chun[1]; Wang Yong[1]; [1]Northeastern University of China

Pure Al matrix foam was fabricated by foaming an Al melt utilizing a newstir method to uniformly mix the foaming agent with the melt.This method was used to address the problems associated with the rapid decomposition of the foaming agent at the hyper-melting point temperature of pure Al. The effect of foaming time on the quality of the pure Al matrix foam material was studied. The optimal processing conditions for fabricating excellent pure Al matrix foam were determined and the compressive properties of the resulting pure Al matrix foam material were measured.

12:10 PM

The Effect of Grain Boundary Character Distribution on the Stress Corrosion Cracking Susceptibility of 2124 Aluminum Alloy: *Lisa Chan*[1]; Anthony Rollett[1]; Gregory Rohrer[1]; Hasso Weiland[2]; Soonwuk Cheong[2]; [1]Carnegie Mellon University; [2]Alcoa Technical Center

Grain Boundary Character Distribution (GBCD) of the 2xxx series aluminum alloys may play a key role in explaining their stress corrosion cracking susceptibility. In the present study, a 2124 aluminum alloy was processed with three different heat treatments and stress corroded according to ASTM G44 standards with 3.5% NaCl solution as a corrosive medium. The recrystallization textures from the three different samples were obtained from X-ray diffraction and automated Electron Back-Scatter Diffraction (EBSD). The following were characterized: statistical 5-parameter GBCD, crack characteristics, electrical conductivity, and hardness. The effects of recrystallization texture and the change in GBCD on stress corrosion cracking susceptibility of 2124 aluminum alloy will be discussed.

Innovations in Electrometallurgy: Session II

Sponsored by: The Minerals, Metals and Materials Society, TMS Extraction and Processing Division
Program Organizers: Adam Powell, Veryst Engineering LLC; Michael Free, University of Utah

Thursday AM — Room: Oceanic 5
March 1, 2007 — Location: Dolphin Hotel

Session Chair: Adam Powell, Veryst Engineering LLC

9:00 AM Invited

Electrochemical Reactors for Metal Recovery from Aqueous Halide Electrolyte Solutions: Chun-yee Cheng[1]; Richard Dawson[1]; *Geoff Kelsall*[1]; Anna Robson[1]; [1]Imperial College London

Applications of electrochemical technology involving low reactant concentrations require electrodes with high mass transport rates and specific surface areas to increase cross-sectional current densities and optimise capital and operating costs. Experimental results will be compared with model predictions for two such reactor types, which facilitate adherent and coherent deposit morphologies: a) cathode feeder electrodes contacting unconsolidated beds of moving, conducting particles that can grow, and enable continual harvesting of the metallic product by hydraulic transport from the bed of the particles; b) mesh cathodes in fluidised beds of inert particles, to enhance mass transport rates; used for metal recovery from: i) low concentrations of platinum in aqueous iodide solutions; ii) acidic aqueous chloride solutions, produced by the leaching of waste electrical and electronic equipment, containing precious metals in low concentrations and base metals in high concentrations.

9:30 AM

An Examination of Ferric Ion Reduction in Sulfate Based Copper Electrowinning Electrolyte: Ravindra Bhide[1]; Jinshan Li[1]; *Michael Free*[1]; J. Miller[1]; J. Brent Hiskey[2]; [1]University of Utah; [2]University of Arizona

An anodic reaction of oxidation of ferrous ions has been proposed as an alternative to water hydrolysis to reduce the cell voltage and power consumption while also eliminating acid mist in the conventional copper electrowinning process. The use of ferrous ion oxidation at the anode results in ferric ions and therefore a corresponding need for reduction of ferric ions to ferrous ions in order to facilitate an acceptable overall process. In this study, different compounds were evaluated as ferric ion reductants. The performance of these compounds was evaluated in relation to overall process requirements.

9:55 AM

The Effect of Organic Additive Properties on Morphology of Copper Electrodeposits from Halide Media: *Aphichart Rodchanarowan*[1]; [1]University of Utah

A decrease of surface roughness in electrodeposits can often be accomplished by the addition of organic additives. The effect of molecular weights, such as glycine monomer, proline monomer, gelatin, polyethylene glycol (PEG, Mw~200 and Mw~10,000), polyethylene oxide (PEO, Mw~300,000), and polyacrylamide (PAA, Mw~200,000) on surface morphology of copper electrodeposit from halide media (0.10 mol/L CuCl, 4.0 mol/L NaCl, and 0.010 mol/L HCl) was studied under current controlled conditions (-25 mA/cm2). Surface roughness was characterized by a series of CCD camera images combined with computer analysis of the images. It was found that the organic additives with high molecular weight (gelatin, PEO, and PAA) gave more uniform deposits compared to those obtained without any additives, yet organic additives with lower molecular weights (PEG) and monomers (glycine and proline) did not significantly reduce the surface roughness.

10:20 AM

Sn(II) Formation by Galvanostatic Electrolysis and Dissolution from Hydrochloric Acid Solution Containing High Concentrations of In(III) and Sn(IV): *Kazuya Koyama*[1]; Mikiya Tanaka[1]; Shinji Fujiwara[2]; Kunio Saegusa[2]; [1]National Institute of Advanced Industrial Science and Technology; [2]Sumitomo Chemical Company, Ltd

The present authors are studying the hydrometallurgical recycling process of indium from an indium-tin-oxide(ITO) target. For this process, in order to obtain the ITO powder with the required properties, the reduction of Sn(IV) to Sn(II) by a combination of the galvanostatic electrolysis and the dissolution of the product from an aqueous hydrochloric acid solution containing high concentration of In(III) and Sn(IV) was examined. As a result, Sn(II) was formed during the electrolysis. This is caused by the electrodeposition of leaf-like tin and dissolution of peeled tin whose reaction was Sn(cathode) + Sn(IV) = 2Sn(II). More than 95% of the Sn(IV) were reduced to Sn(II) by the electrolysis such as half of the Sn(IV) in the solution was theoretically deposited, and the dissolution.

Innovations in Titanium Technology Symposium: Microstructure and Properties II

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS: Titanium Committee
Program Organizers: Mehmet Gungor, Concurrent Technologies Corporation; M. Ashraf Imam, Naval Research Laboratory; F. H. (Sam) Froes, University of Idaho

Thursday AM — Room: Asia 3
March 1, 2007 — Location: Dolphin Hotel

Session Chairs: Ibrahim Ucok, Concurrent Technologies Corporation; Catherine Wong, Naval Surface Warfare Center

9:00 AM Invited

Crack Growth, Microstructure and Texture in Ti-6Al-4V: David Dye[1]; *Ioannis Bantounas*[1]; Trevor Lindley[1]; [1]Imperial College

The effect of local texture on fatigue damage has been examined in Ti-6Al-4V. Fatigue performance has been found to be heavily dependent on the orientation of basal planes to the loading axis. The present study employs EBSD to determine the orientation of grains surrounding an arrested crack in three Ti-6Al-4V product forms. Schmid factor calculations have been made to establish the preferred slip system active in the grains surrounding the crack. It is shown that for all three materials cracks have arrested at grains favourably oriented for <c+a> slip (1st and 2nd order pyramidal slip). The operating

slip modes were found using TEM foils removed using the FIB technique. The resistance to fatigue crack development is found to be dependent on the probability of a nucleated crack interacting with grains oriented for <c+a> slip, as well as the ease by which a crack can pass around such a grain.

9:30 AM
Probabilistic Sensitivity Analysis of the Life-Limiting Mechanism in an α+β Titanium Alloy and Application to Fatigue Life Prediction: *Sushant Jha*[1]; Harry Millwater[2]; James Larsen[3]; [1]Universal Technology Corporation; [2]University of Texas, San Antonio; [3]US Air Force

The total uncertainty in lifetime of the α+β titanium alloy, Ti-6Al-2Sn-4Zr-6Mo, could be described as a superposition of variability in the life-limiting and the mean-lifetime controlling behavior. Additionally, the variability in the life-limiting mechanism was governed by crack growth starting from an equiaxed α grain. A probabilistic sensitivity analysis was developed to study the effect of the parameters of the controlling random variables on the life-limiting mechanism. In particular, expressions for sensitivity of response mean and standard deviation for correlated and independent random variables were derived and applied to rank the parameters impacting the minimum lifetime and the variability in the worst-case mechanism. The sensitivity regimes developed here can be implemented in a life-prediction methodology that may enhance the useful capability of titanium alloys in fracture critical applications.

9:50 AM
The Mean vs. Life-Limiting Behavior in Fatigue of an α+β Titanium Alloy: *Sushant Jha*[1]; James Larsen[2]; Reji John[2]; Andrew Rosenberger[2]; [1]Universal Technology Corporation; [2]US Air Force

The mean and the life-limiting behavior in fatigue of the α+β titanium alloy, Ti-6Al-2Sn-4Zr-6Mo, responded differently to stress level, microstructure, and temperature. This dual response was related to the dependence of the life-limiting and the mean-lifetime dominating mechanism on crack growth, and crack initiation respectively. The different degree of sensitivity of the two fatigue regimes to these variables produced the separation of responses. This behavior was studied, both in the presence and absence of surface residual stress. An alternate paradigm of fatigue variability behavior was developed, that accounts for the mean-lifetime vs. the life-limiting behavior and implemented in a life-prediction approach. The approach was validated by a physically-based probabilistic lifetime simulation. The significance of the alternate theory as opposed to the traditional mean-lifetime based understanding of the fatigue variability behavior, for reduction in the uncertainty in design life and life-management of fracture critical components will be discussed.

10:10 AM
High Temperature Oxidation of Ti3Al-4at%Nb Alloys: *Chris Williams*[1]; Ramana Reddy[1]; [1]University of Alabama

The Oxidation studies on Ti3Al-4.0at%Nb samples were carried out in pure oxygen atmosphere at temperatures ranging from 1023-1373 K using Thermogravimetric Analysis (TGA) apparatus. Samples were characterized using scanning electron microscopy (SEM), X-ray diffraction (XRD), and electron-dispersive X-ray (EDX). Reaction products consisted of rutile and alumina particles. From the weight gain measurements, the reaction rate constants as a function of temperatures were determined. Effective activation energy of 222 kJ/mol was determined. This composition shows increased oxidation resistance over comparable binary Ti3Al compositions. The results are compared and discussed with the available literature data on Ti-Al-Nb alloys.

10:35 AM Break

10:50 AM
Evaluation of TiN Coatings Produced via Different Techniques: *Ali Arslan Kaya*[1]; Selda Ucuncuoglu[1]; Kerim Allahverdi[1]; [1]TUBITAK-Marmara Research Center

TiN coatings were created on Ti-6A-l4V substrate using two different techniques, namely PVD and heat treatment under controlled atmosphere. The aim was to choose one of these techniques to employ for creating TiN deposits of known size, shape and location on the surface of a titanium alloy block. This surface was later to be bonded to another titanium alloy block via diffusion bonding, thus encapsulating the TiN deposits in the metallic body. Such titanium bodies carrying TiN as synthetic defects can be used as calibration blocks in ultrasonic inspection of titanium alloy parts in aircraft industry. The TiN coatings produced via two methods were characterized using Confocal Raman, Atomic Force Microscopy (AFM), XRD, scratch test as well as scanning electron microscopy (SEM) techniques.

11:10 AM
Some Engineering Aspects of Thermohydrogen Treatment of Large Complex Titanium Alloy Castings: *Guoping Cao*[1]; Hai Nan[2]; Chengmu Xie[2]; [1]University of Wisconsin; [2]Beijing Institute of Aeronautical Materials

Thermohydrogen treatment is an effective method to improve the mechanical properties of titanium alloy castings. In this paper, some engineering aspects of thermohydrogen treatment of large complex Ti alloy castings were discussed. From the point of engineering application, the effects of thermohydrogen treatment were studied on the overall mechanical properties including room temperature tensile strength, 350°C tensile strength, 350°C durability, room temperature fatigue strength and fracture toughness. The feasibility of applying thermohydrogen treatment to large thick-walled (up to 45mm wall thickness) titanium casting was also studied. Some real Ti alloy castings were tested using thermohydrogen treatment. Our results showed that thermohydrogen treatment was very suitable to heat treat the large complex titanium castings when high temperature endurance and fatigue strength are desired or required.

11:30 AM
Flame Spray Welding of NiCrBSi Powder Alloy on Titanium Alloy Substrate: *Xiaojing Xu*[1]; [1]Jiangsu University

The present paper deals with a study of flame spray welding of NiCrBSi powder alloy on titanium alloy (Ti-6Al-4V) substrate. In order to overcome the harmful effect of titanium oxide to coating, prior to the spraying a surface pretreatment consisting of ion etching and subsequent electroless deposition of zinc was carried out. In order to increase the diffusion of elements, the time for the coating to stay at liquid state was appropriately lengthened. Due to these modifications, a high quality coating with the thickness of about 1 mm was successfully developed. This coating presented many characterization, such as little pore and inclusion, smooth change in elements distribution and microstructures, good metallurgical bonding in interface, and very high wear-resistance as the result of diffusion of Ti element up to the top layer of the coating.

Magnesium Technology 2007: Corrosion and Coatings

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Magnesium Committee
Program Organizers: Randy Beals, DaimlerChrysler; Neale Neelameggham, US Magnesium LLC; Mihriban Pekguleryuz, McGill University; Alan Luo, General Motors Corporation

Thursday AM Room: Southern 4
March 1, 2007 Location: Dolphin Hotel

Session Chairs: Neale Neelameggham, US Magnesium LLC; Robert McCune, Ford Motor Company

9:00 AM
The Influence of De-Icing Salts on Corrosion of Mg Alloys: Okechukwu Anopuo[1]; Carsten Blawert[1]; *Norbert Hort*[1]; Karl Kainer[1]; [1]GKSS Research Center

The seasonal application of de-icing salts on the roads in the northern hemisphere during winter to prevent icing of roads and for snow removal possesses threat not only to shrubs by the road sides but also to certain engineering metals used in our automobiles. In this work, the corrosive effect of these salts on standard commercial magnesium alloys was examined. Immersion tests were carried out with NaCl, CaCl2 and MgCl2 solutions. Mixtures of NaCl, MgCl2 and between 10wt.-% to 50wt.-% of CaCl2 were used for immersion tests, and their influence on the corrosion behaviour of the chosen magnesium alloys was studied. Additionally, electrochemical tests were carried out in order to gain insight into the hydrogen evolution of these engineering materials in different salt solutions.

9:20 AM

Characterisation of the Corrosion Behaviour of Mg and Its Alloys with the Mini Cell System: *Claudia Fleck*[1]; M. Lucia Nascimento[1]; Wolf-Dieter Mueller[2]; [1]Technical University of Berlin; [2]Charité Berlin

The electrochemical behaviour of magnesium and different wrought alloys, AZ31, AE42, LAE442, and ZEK100, with and without heat treatment, was examined with the Mini-cell System by linear sweep voltammetry in 0.5 wt.-% and 3.5 wt.-% NaCl solution. The corrosion damage was characterised by scanning electron microscopy. Magnesium and the different alloys exhibited strong differences in their electrochemical behaviour. Alloying with aluminium increases the corrosion resistance. However, the magnitude of this improvement depends on uniform sizes and distributions of the Al-rich phases. Similarly, the influence of the heat treatment on the corrosion resistance depends on the produced distribution of precipitates. Magnesium and its alloys corrode quite rapidly in comparison with other metals, and there is a pronounced hydrogen development. The latter increased with increasing NaCl concentration, although no great differences in the corrosion in both concentrations were observed, except on pure magnesium and ZEK100.

9:40 AM

Film Formation on Magnesium Alloys in Aqueous Solutions and Detection by Rutherford Backscattering Spectroscopy: *Robert McCune*[1]; Deepan Sivaraj[2]; Pankaj Mallick[2]; Zhiming Shi[2]; [1]Ford Motor Company; [2]University of Michigan-Dearborn

Rutherford Backscattering Spectroscopy (RBS) has been used previously for assessment of film formation and understanding protective mechanisms for aluminum alloys exposed to automotive engine coolants. The technique permits a rapid comparison of inhibitor anion interactions with the metal surface, and measurement of the extent of hydrated oxide development. A similar approach has been devised for magnesium alloys in anticipation of their potential use for the cylinder blocks of lightweight, water-cooled internal combustion engines. This presentation firstly reviews the fundamentals of the technique and secondly presents initial findings on aqueous film formation and DC electrochemical polarization of pure magnesium in the presence and absence of protective film-stabilizing additives to aqueous solutions.

10:00 AM

Boron-Based Lubricants for Magnesium in Transportation and Manufacturing Applications: *Ali Erdemir*[1]; Oyelayo Ajayi[1]; George Fenske[1]; [1]Argonne National Laboratory

Because of their very high strength-to-weight ratios, magnesium and its alloys have generated huge interest from automotive and related industries. However, these materials are difficult to manufacture into useful automotive parts and when used as a tribological components (i.e., engine blocks), magnesium is not responding well to current lubricants thus leading to high friction and wear losses. In this paper, we will introduce a range of novel boron-based solid and liquid lubricants that can resolve most of the lubrication problems experienced with magnesium during manufacturing as well as tribological sliding. With the uses of boron-based lubricants, we observed significant reductions in friction (as high as 80%) and wear (more than 90%). Detailed surface studies after the tests confirmed the formation of a strongly bonded boron-rich boundary film on sliding surfaces which seems to confirm that these lubricants are very responsive and compatible with magnesium and its alloys.

10:20 AM Break

11:00 AM

Zinc-Calcium-Manganese Phosphate Chemical Conversion-Coating Treatment for Magnesium Alloys: Yongfeng Jiang[1]; *Yefeng Bao*[1]; [1]Hohai University

The zinc-calcium-manganese phosphate conversion coating for AZ91D magnesium alloy are studied. The adhesive strength is investigated by alcohol rubbing test. The salt spray tests and polarization curves are used to test the corrosion resistance of the coating in 5% NaCl solution, and the electrical conductivity is also measured by mini-Ohm meter. Zinc-calcium-manganese phosphoric chemical conversion coating is compact and its adhesive strength attains to IBM standard. The Salt Spray of coating is evaluated above B class and 9 levels according to ASTM B117. Polarization curve reveals that the anti-corrosion of the magnesium after phosphate treatment is better than the magnesium substrate. After phosphate chemical conversion coating, the electrical conductivity is between 0.015~0.068 Ohm.

11:20 AM

Influence of Pulse Frequency on Plasma Electrolytic Oxidation Processes of Mg Alloy Surface: *Zhenmin Liu*[1]; Tian Qiu[1]; Wei Gao[1]; [1]University of Auckland

Process of plasma electrolytic oxidation (PEO) of magnesium alloy AZ91 in an electrolyte containing sodium hydroxide and sodium phosphate was investigated. The effect of electrical pulse frequency on the process of plasma electrolytic oxidation under bipolar polarization modes was also discussed. It was found that increase in pulse frequency leads to reduced porosity, improved uniformity and corrosion resistance of the formed layer. This is attributed to the increase in number of micro-discharges and the reduction in the discharge size on the article surface. The improved uniformity of the PEO coating could be explained by the effect of skin effect and the resultant intensification of plasma chemical synthesis processes. A physical and numerical model has been established to connect the formed coating thickness with relevant physical parameters. Optimal combination of the electric pulse frequency and the duty ratio for corrosion resistance appeared to be 500 Hz and 50%, respectively.

11:40 AM

Surface Modification of Magnesium by Micro Arc Oxidation: *Murat Baydogan*[1]; Mert Gunyuz[1]; Huseyin Cimenoglu[1]; Eyup Kayali[1]; [1]Istanbul Technical University

In this study, commercially pure magnesium having dimensions of 10 x 20 x 5 mm was oxidized in an alkali solution for 30 min on a 30 kW AC micro-arc oxidation equipment. Characterization of the oxidized surfaces was made by microstructural analysis, roughness measurements, hardness measurements, scratch and wear tests. Microstructural investigations performed on the surfaces and cross sections of the samples by X-ray diffraction analysis and microscopic examinations revealed that oxide layer, which was mainly consist of magnesium oxide, was compact and dense. Formation of oxide layer by micro-arc oxidation on magnesium resulted in considerable surface hardening and surface roughing. The results of the scratch tests showed that that oxide layer was reasonably tough. Reciprocating wear tests revealed that micro-arc oxidation caused considerable improvement in wear resistance when compared to unoxidized state.

12:00 PM

Coating Adhesion for Mg Alloy ZE41A: *Richard Griffin*[1]; David Zuniga[1]; Milli Datta[1]; [1]Texas A&M University

Mg ZE41A is a castable alloy that has applications in helicopters. It is light weight and has very good stiffness. Mg alloys are active metals and must be protected to be used safely. The alloy ZE41A was tested with a green coating and compared to a chromate containing anodic coating. The coating combinations were tested in JP8, distilled water, Royco 555 aviation hydraulic fluid and Royco 787 turbine lubricating oil The combinations were anodic coating, anodic coating plus epoxy, anodic coating plus epoxy plus primer and anodic coating plus epoxy plus primer plus top coat. A hydraulic pull-off adhesion tester was used to determine the force required. We will discuss the results and compare the adhesion values. There were substantial differences for the same coating. We used an Anova table to draw correlations between the coating system tested and the medium the coating system was tested in.

12:20 PM

Nondestructive Evaluation of an Environmentally Friendly Conversion Coating for Magnesium Alloys Using an Infrared Proximity Sensor and Polarized Light Microscopy Techniques: *David Zuniga*[1]; Richard Griffin[1]; [1]Texas A&M University

Magnesium alloys have one of the highest specific strengths of all construction materials used. Although magnesium alloys provide additional desirable traits such as high damping capacity, reduced tool wear and lower melting temperatures for ease of recycling, they are also the most prone to corrosion when compared to all construction materials [R. S. Busk, Magnesium Products Design (Mercel Dekker, Inc, New York, 1987)]. Anti-corrosion coating systems allow the use of magnesium alloys in harsh environments, as in the case of the H-60 helicopter magnesium alloy gearbox housing. However, the conversion coating which forms the foundation of many of these coating systems employs chromium. In an effort to phase these harmful chromates out of the coating system and continue to use magnesium alloys, an

environmentally friendly conversion coating has been developed. This paper shall present data acquired from an infrared proximity sensor which shows the difference between an environmentally friendly coated magnesium alloy ZE41A and uncoated ZE41A to establish a measure of quality control for the environmentally friendly coating. This paper shall also present data acquired using traditional polarized light microscopy techniques to determine the difference between a coated and uncoated magnesium alloy using mean gray value counting to achieve the same goal as the infrared sensor experiment.

Magnesium Technology 2007: Microstructure and Properties

Sponsored by: The Minerals, Metals and Materials Society, TMS Light Metals Division, TMS: Magnesium Committee
Program Organizers: Randy Beals, DaimlerChrysler; Neale Neelameggham, US Magnesium LLC; Mihriban Pekguleryuz, McGill University; Alan Luo, General Motors Corporation

Thursday AM Room: Southern 5
March 1, 2007 Location: Dolphin Hotel

Session Chairs: Norbert Hort, GKSS; Eric Nyberg, Pacific Northwest National Laboratory

9:00 AM
The Determination of Hall-Petch Constants in Pure Mg: *Gemma Mann*[1]; Carlos Caceres[1]; John Griffiths[2]; [1]University of Queensland; [2]CSIRO

Flow stress data from specimens tested in tension or compression, with grain sizes ranging from 90 µm to 1440 µm have been used to construct Hall-Petch plots. Three different methods were used to obtain the yield strength data: 0.2% offset proof stress; finding the minimum of the second derivative of the flow stress with respect to the strain; and the stress at which the strain after unloading is 0.2%, thus subtracting the pseudoelastic component of the strain introduced by twinning. It is shown that the last method leads to more self-consistent results. It is also shown that the usual method of finding the Hall-Petch constants through linear regression may sometimes lead to negative values of the friction stress. It is argued that the friction stress should be introduced as a physical constant, calculated from first principles, in order to obtain more reliable values for both the friction stress, σ_o, and the stress intensity parameter, *k*.

9:20 AM
3D Characterization of Beta-Phases AZ91D by Synchrotron-Radiation Based Microtomography: Frank Witte[1]; Jens Fischer[2]; Michael Störmer[2]; *Norbert Hort*[2]; [1]Hannover Medical School; [2]GKSS Research Center

The beta phase Mg17Al12 influences high temperature strength as well as corrosion properties of Mg-Al alloys. Mg17Al12 develops during casting and its morphology depends also on heat treatments and processing. Normally the beta phase, its morphology and distribution is determined by standard metallographic methods leading only to a two dimensional picture. Synchrotron-radiation based microtomography (SRµCT) is able to give a 3D image of the microstructure and is used here to characterize the distribution of Mg17Al12 in as-cast and extruded AZ91D. The synchrotron radiation based results have been supplemented by XRD and methods of metallography.

9:40 AM
Threshold Stress during Tensile and Compressive Creep in AE42 Magnesium Alloy: *Hajo Dieringa*[1]; Norbert Hort[1]; Karl Ulrich Kainer[1]; [1]GKSS Research Center

The use of magnesium alloys in engine or powertrain applications is one of the greatest challenges in development of light weight magnesium alloys. Whereas room temperature applications are already in use for a long time for example in steering wheels, inner door frames or steering columns, components with service temperatures of more than 150°Crequire specific strength and creep resistance. Aluminum and rare earth containing magnesium alloy AE42 is expected to be a candidate for such applications. High creep resistance is attributed to AlRE-precipitates which form during solidification. Tensile and compressive creep tests are performed at temperatures between 150°Cand 200°Cwith applied stresses between 40 and 100 MPa. In this investigation the influence of direction on the minimum or secondary creep rate is examined. Additional analysis of creep rates in terms of determining deformation mechanisms during creep are investigated in this paper.

10:00 AM
Analysis of the Creep Response of the AE44 Magnesium Alloy between 100 and 150°C: *Enrico Evangelista*[1]; Stefano Spigarelli[1]; Mohamad ElMehtedi[1]; Marcello Cabibbo[1]; [1]University of Ancona

The creep response of the AE44 magnesium alloy was investigated by means of constant load creep tests carried out between 100 and 150°C. The minimum creep rate dependence on applied stress was described by a conventional power law, with a stress exponent n larger than 30 at the highest temperature. The minimum creep rate in the low stress regime was thus about two orders of magnitude lower in AE44 than in AM50. This large difference in creep response has been attributed to the presence and evolution of rare earths (RE) intermetallic phases mainly distributed in the grain boundary zone in form of an almost continuous network of dispersoids, that were observed by means of optical and scanning electron microscopy.

10:20 AM
Creep Behavior of Permanent Mold Cast Mg-Al-Ca Based Alloys: *Nicholas Saddock*[1]; Akane Suzuki[1]; Jessica TerBush[1]; Tresa Pollock[1]; Wayne Jones[1]; [1]University of Michigan

The creep behavior of AX44 (Mg-4Al-4Ca) and AXJ530 (Mg-5Al-3Ca-0.15Sr, wt%) was investigated in permanent mold cast alloys at stresses ranging from 60 to 100 MPa and temperatures from 398 to 498 K. A strain mapping technique was used to investigate deformation, using a periodic array of micron-scale markers deposited on the specimen surface. By measuring changes in array spacing as a function of creep strain a two-dimensional strain field is calculated at the specimen surface. In this study strain distributions during creep were investigated with particular attention given to assessing the role of microstructure. Out-of-plane deformation was also quantified by analysis of stereo pair images and mathematical reconstruction of the topography of the surface. Evidence for strain localization and comparison with deformation on the scale of the dendritic cells and grains for the alloys investigated is described and discussed.

10:40 AM Break

11:00 AM
Microstructure Study of Pure Mg and Mg-Al at Various Stages of Creep Using EBSD: *Takanori Sato*[1]; Barry Mordike[2]; Jian-Feng Nie[3]; Milo Kral[1]; [1]University of Canterbury; [2]Institut für Werkstoffkunde und Werkstoftechnik, TU Clausthal; [3]Monash University

Magnesium and common Mg-Al based alloys typically exhibit constant creep rate during secondary creep stage, described as power law creep. Diffusion induced dislocation motion and grain boundary sliding is known to be the key to understanding the mechanisms of creep in magnesium. Furthermore, with addition of aluminum, the coarse intergranular and fine coherent intragranular ß (Mg17Al12) precipitates are known to affect the creep rate. In this research, 99.96% wrought magnesium and diecast AZ91 alloys were tested for tensile creep at various conditions ranging from 100 to 200°C. The tests were interrupted periodically and sample surface microstructure was analyzed using SEM/EBSD (electron backscatter diffractography) providing sequential microstructure analysis of identical sample surface locations at various stages of creep. Observations involving the initial stress relaxation and gradual formation of low angle boundaries expand the understanding of the contribution of dislocation accumulation and grain boundary slide to the creep of magnesium.

11:20 AM
Microstructure and Hardness of Mg-Sn-Zn Alloys with Various Heat Treatments: *Taisuke Sasaki*[1]; Keiichiro Ohishi[2]; Tadakatsu Ohkubo[2]; Toshiji Mukai[2]; Kazuhiro Hono[2]; [1]University of Tsukuba; [2]National Institute for Materials Science

To explore the possibility of the development of heat treatable wrought magnesium alloys, we have investigated the age hardening behavior of Mg-Sn based alloys. The addition of 0.5at.%Zn was found to enhance the peak hardenss of Mg-2.2at.%Sn alloys from 60HV to 73HV by aging at 200°C. Preaging for 24 h at 70°C before artificial aging at 200 °C further enhanced the hardness of the Mg-2.2Sn-0.5Zn to 80 HV. Increased number density and refinement

of lath-shaped $MgSn_2$ precipitate are attributed to the enhanced hardening. The solution treated Mg-2.2Sn-0.Zn alloy was found to be cold rolled up to 50% reduction in thickness and its hardness was 86 HV. By artificially aging solution-treated cold rolled samples, moderate age hardening was observed after slight reduction in hardness due to recovery. The microstructure of these cold rolled age hardened alloys showed much finer microstructure composes of spherical precipitates.

11:40 AM

Aging Characteristics and Mechanical Properties of Cast and Wrought Mg-11Gd-2Nd-0.5Zr Alloys: *Kaiyun Zheng*[1]; Jie Dong[1]; Xiaoqin Zeng[1]; Wengjiang Ding[1]; [1]Shanghai Jiao Tong University

In this work, the aging characteristics and mechanical properties are investigated for Mg-11Gd-2Nd-0.5Zr alloy in cast or wrought condition. A noticeable temperature dependence of age-hardening response is recognized in alloy after solution treatment, and the tensile properties of peak-aged alloy changes with different aging temperatures. With heat treatment consisting of solution at 525°C for 4h and aging at 250°C for 2h, the alloy exhibits high strength at temperature up to 300°C. Cold work of 10% stretching or rolling deformation prior to aging causes acceleration of age-hardening response without increasing the maximum hardness. Combined action of cold deformation and aging improves the strength but worsens the ductility. Effective grain refinement is achieved by hot extrusion at 450°C, resulting in high strength and moderate ductility for as-extruded alloy. Hot extrusion accelerates the age-hardening response and increases the maximum hardness. Subsequent aging further improves the strength but deteriorate ductility of the as-extruded alloy.

12:00 PM

Microstructural Investigations of Mg-Al Alloys Containing Small Amounts of SiC Nucleants: *Yuanding Huang*[1]; Norbert Hort[1]; Okechukwu Anopuo[1]; Gabriele Vidrich[2]; Andreas Schiffl[3]; Yi-Lin Liu[4]; [1]GKSS Research Centre; [2]Clausthal University of Technology; [3]ARC Leichtmetallkompetenzzentrum Ranshofen GmbH; [4]Risø National Laboratory

Previous investigations indicated that addition of SiC can be used for grain refinement in Mg-Al alloys. In this work the microstructure of Mg-Al alloys containing small amounts of SiC particles is investigated with an emphasis on the interactions among Mg, Al and SiC. It was found that the amount of SiC particles largely decreases after casting. SEM and XRD experiments show the existence of Mg17Al12 and Mg2Si phases. The chinese script-like Mg2Si particles are surrounded by Mg17Al12 which is normally located at the dendritic grain boundaries. An analysis of the composition showed a carbon enrichment at the grain boundaries. In addition, some micro-cracks were observed close to the grain boundaries. All these phenomena illustrate the occurrence of interactions among Mg, Al and SiC. Based on these results, the effects of these interactions on the grain refinement are discussed for Mg-Al alloys.

12:20 PM

The Microstructural Evolution of Hot Worked and Annealed Magnesium Alloys: Aiden Beer[1]; *Matthew Barnett*[1]; [1]Deakin University

The microstructural evolution during the annealing of hot worked magnesium alloys is examined. Firstly, the influences of deformation and annealing conditions on the developed microstructures are assessed. Static recrystallization of the dynamically recrystallized structure occurs, with the stable annealed grain size being governed solely by the prior deformation conditions employed. With increasing values of Z (higher strain rates and lower temperatures), smaller annealed grain sizes are attained and the time at which coarsening begins reduces. The influence of alloy addition on the annealing behaviour is examined for the AZ and ZK alloy series. With increased alloy levels, the annealed grain size is reduced. Of the additions studied, Zr was most effective in reducing the annealed grain size.

12:40 PM

Mechanical Properties and Texture of Hot Extruded Magnesium Alloys via RCP Process in Using Coarse Raw Powder: *Katsuyoshi Kondoh*[1]; Kenshi Kawabata[1]; Hideki Oginuma[1]; [1]Osaka University

Roll Compaction (RCP) process consisting of twin rolls, is available to assist the grain refinement and texture control of coarse magnesium alloy powders by applying severe strain hardening to them by all direction. Wrought magnesium alloys consolidated by hot extrusion in employing RCPed powder show a good balance of tensile strength and elongation. For example, in applying RCP process to AZ31 alloy, the extruded one reveals TS of 380 MPa, YS of 310 MPa and 15% elongation at room temperature, Grain growth could be also controlled by refined oxide dispersoids in the matrix during annealing at 673K for 3.6 ks. EBSP analysis concerned that RCP accelerated not only grain refinement but texture control, that is, the activation of basal and nonbasal dislocations.

Materials in Clean Power Systems II: Fuel Cells, Solar, and Hydrogen-Based Technologies: Materials for Solar Cells and Photovoltaic Systems

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

Program Organizers: Zhenguo "Gary" Yang, Pacific Northwest National Laboratory; Michael Brady, Oak Ridge National Laboratory; K. Scott Weil, Pacific Northwest National Laboratory; Yong-Ho Sohn, University of Central Florida

Thursday AM — Room: Asia 2
March 1, 2007 — Location: Dolphin Hotel

Session Chairs: Beatriz Cuenya, University of Central Florida; Prabhat Kumar, HC Starck Inc

9:00 AM Invited

Routes to Formation of $CuIn_xGa_{1-x}Se_2$ Thin Film Absorbers for Photovoltaics: *Timothy Anderson*[1]; Woo Kyoung Kim[1]; Suku Kim[1]; Seokhyun Yoon[1]; Chih-Hung Chang[2]; Jianyun Shen[1]; E. Andrew Payzant[3]; [1]University of Florida; [2]Oregon State Unversity; [3]Oak Ridge National Laboratory

Chalcopyrite Cu(In,Ga)Se2 is one of the most promising absorber materials for high efficiency thin film solar cells with reported conversion efficiency approaching 20%. Central to lowering the cost of cells is developing routes to formation of this material at high rates and low temperature. To better understand growth of this material a systematic assessment of the phase diagram of this 4 component system has been performed. In addition, a systematic study of the reaction pathways and kinetics for the formation of $CuIn_xGa_{1-x}Se_2$ thin films was performed using in-situ high temperature X-ray diffraction. Reaction pathways under both inert and Se overpressure were examined for a variety of elemental and bilayer precursor film structures and kinetic analysis of the data allowed mechanism differentiation and rate parameter estimation. The observed pathways are compared to those suggested by diffusion limited transport with equilibrium conditions at the interfaces.

9:35 AM

Electrical and Structural Properties of Nanocrystalline Silicon Intrinsic Layers for Nanocrystalline Silicon Solar Cells Prepared by Very High Frequency Plasma Chemical Vapor Deposition: *Prabhat Kumar*[1]; Feng Zhu[1]; Josh Gallon[2]; Arun Madan[3]; [1]Colorado School of Mines; [2]MVSystems Inc.; [3]MVSystems Inc. and Colorado School of Mines

Nanocrystalline silicon intrinsic layers were deposited to investigate their structural and optoelectrical properties using very high frequency PECVD. The typical SiH* and Ha intensity at ~414 and ~656 nm from optical emission spectroscopy increase with the plasma power 5-50 W. The films are nanocrystalline at low SiH*/Ha ratio as it exhibits two crystalline peak in reflectance spectra at ~275 and ~350 nm. The crystalline fraction is ~40-70% exhibiting photosensitivity of 10-1000. The SiH mode at 2000 cm-1 gets converted into SiH or SiH2 mode at 2100 cm-1 as the materials changeover from amorphous to nanocrystalline. The SiH* and Ha intensity decrease as the pressure is increased from 200 mTorr to 1000 mTorr at constant power 15W. The films were nanocrystalline in this pressure range. The photosensitivity is in the range of 10-10000 depending on the crystalline fraction in the film. The solar cell results will be presented at the conference.

10:00 AM
Novel Materials for Use as Photoelectrodes for Hydrogen Production in Photoelectrochemical Cells: *Alex Stavrides*[1]; Augusto Kunrath[1]; Jian Hu[1]; Richard Treglio[2]; Ari Feldman[2]; Bjorn Marsen[3]; Brian Cole[3]; Eric Miller[3]; Arun Madan[1]; [1]MVSystems, Inc.; [2]Colorado School of Mines; [3]Hawaii Natural Energy Institute

We have previously reported on an integral "hybrid" photoelectode which would lead to >3% solar-to-hydrogen conversion efficiency (STH). The device configuration consisted of stainless steel/a-Si(nipnip)/ZnO/WO3 immersed in an electrolyte. The efficiency of this device, in its present form, is limited by the photocurrent produced by the WO3 photoanode, as the bandgap is ~2.6eV. Utilizing a photoelectrode with a reduced bandgap of ~2.3 eV (and other suitable properties) would increase the photocurrent, thus leading to a theoretically achievable STH above the performance target of 10% set by the United States Department of Energy. We will report on growth of a-SiC, a-SiNx, and Cu-doped ZnO, and characterization of the properties of these films, such as photoconductivity, photocurrent, and band-edge positions, which are relevant to their performance as photoelectrodes. Finally, we will report on devices which include these new materials, and our progress toward the 10% STH goal.

10:25 AM
Novel Titania Based Photo Anodes with Increased Photo Catalytic Activity for Water Splitting: *Vishal Mahajan*[1]; Krishnan Raja[1]; Manoranjan Misra[1]; [1]University of Nevada

Present work was designed to study the use of hybrid TiO2 nanotubular arrays for photocatalytic water splitting. Self ordered titania nanotubes were prepared by the anodization technique. A new way to increase the photocatalytic activity of this semiconductor material by gold nanoparticles (Au-TiO2) and carbon (C-TiO2) incorporation was demonstrated. C-TiO2 was synthesized by two different techniques. In the first technique, carbon was incorporated by using a CVD furnace, and acetylene gas was used as a carbon source in reducing environment. In another technique the carbon deposition was done by anodizing Titanium in organic based electrolyte. Gold incorporation was done by using the sputtering technique. C-TiO2 photoanodes showed photocurrent of 3 mA/cm2 under the illumination of uv+visible light. This photocurrent density corresponds to hydrogen evolution rate of 11 liters/hr on a photo-anode with 1 m2 area. Photocurrent was found to increase in proportion to the increased area of the photo anode.

10:45 AM
Preparation of Highly Efficient Nanocrystallized Photocatalysts for the Production of Hydrogen from a Solar Powered Thermochemical Water Splitting Cycle: *Cunping Huang*[1]; Nazim Muradov[1]; Ali T-Raissi[1]; [1]Florida Solar Energy Center

Solar powered hydrogen production from water splitting is an ultimate goal for hydrogen economics. Different from nuclear heat and other thermal energy sources, solar energy is a renewable energy source and consists of about 33% photonic energy and the rest of thermal heat. The utilization of both energies will enhance the efficiency of hydrogen production. Florida Solar Energy Center has developed a state-of-the-art solar powered sulfur-ammonia thermochemical water splitting cycle for the production of hydrogen, in which solar photonic energy is utilized for the production of hydrogen while solar thermal energy is utilized for the production of oxygen. The objective of this research is to develop a novel approach for the preparation of efficient nanoscaled photocatalysts for the oxidation of aqueous ammonium sulfite solution in the new cycle. Experiments have been carried out and the results are reported in terms of catalyst preparation, structural analyses, and reaction activities.

Materials Processing under the Influence of External Fields: Session V

Sponsored by: The Minerals, Metals and Materials Society, TMS: Aluminum Committee, TMS: Magnesium Committee, TMS: Solidification Committee
Program Organizers: Qingyou Han, Oak Ridge National Laboratory; Gerard Ludtka, Oak Ridge National Laboratory; Qijie Zhai, Shanghai University

Thursday AM Room: America's Seminar
March 1, 2007 Location: Dolphin Hotel

Session Chairs: Edward Ripley, BWXT Y-12 National Security Complex; Dinesh Agrawal, Pennsylvania State University

9:00 AM Introductory Comments

9:05 AM Invited
"Who Says You Can't Microwave a Fork?" - Microwaving Metal Processing at Y-12: *Edward Ripley*[1]; [1]BWXT Y-12 National Security Complex

Over the past decade, techniques for melting, casting and heat-treating metals using microwave energy have been developed. This year microwave metal processing has moved beyond the laboratory and into a larger arena. To date Steels, Platinum, Titanium, Zirconium, Copper, Brass, Bronze, Aluminum, and many others have been melted. Melts exceeding 750 pounds with melting point temperatures in excess of 2675°C have been accomplished and additional scale-up is being pursued. The equipment has a relatively small footprint and is easily converted to a variety of casting setups, material type and atmospheres. This basic method can be used in a variety of metal processing applications. It has been used to melt, cast, heat-treat, sinter, infiltrate, and initiate and carry out chemical reactions.

9:35 AM
On the Effect of Applied Microwave Energy on the C-Co-W Phase Diagram: *Michael Gao*[1]; Anthony Rollett[1]; [1]Carnegie Mellon University

It was reported [Mat. Sci. Eng. A 391 (2005) 285–295] that microwave processing promotes significant W depletion in the Co binder phase in a W-C-Co alloy if compared with conventional sintering process for the same alloy. In this study, we will use CALPHAD approach to study how microwave processing can change the thermodynamics and the phase relationships of this industrially important system. We then extend our study into phase equilibria and solute segregation anisotropy of Fe-1wt%Si under applied magnetic field on a continuum model. This model then is used to predict grain growth behavior of this alloy under applied magnetic field.

10:00 AM Invited
Atmoplas™: A New Microwave Process: *Satyendra Kumar*[1]; D. Kumar[1]; R. Peelamedu[1]; M. Demchak[1]; D. Seccombe[1]; [1]BTU International

Microwaves, at atmospheric pressure, have been used in the past in some industrial applications such as drying and sintering of ceramics etc. These applications have been limited mostly to non-metallic materials due to very small skin depth for metals at microwave frequencies resulting in very little absorption of energy. Conventional microwave techniques use susceptors to address this problem but susceptors are poor absorbers of microwaves at room temperature and take longer to reach the required processing temperatures. A new microwave process, Atmoplas, has been developed at atmospheric pressure that is independent of the nature of material and therefore quite versatile. Recent results of some of the heat treat applications (carburization, sintering, nitriding etc.) will be presented and current efforts in the area of hard materials coatings will be discussed.

10:30 AM Invited
Materials Processing in Microwave E and H Fields: *Dinesh Agrawal*[1]; Jiping Cheng[1]; Y. Fang[1]; R. Roy[1]; [1]Pennsylvania State University

Microwave energy has been in use for quite some time in materials processing including calcinations, drying, synthesis, sintering, melting and brazing etc. Microwave materials processing is well recognized for exhibiting abnormal reaction kinetics in many systems and enhanced material diffusion during sintering. Recently using a 2.45 GHz, single mode microwave cavity, it

is possible to separate E and H components of microwave radiation and expose small size samples in almost pure E and H fields. This presentation will review the research conducted under separate E and H fields at 2.45 GHz. The survey of variety of samples of metals, ceramics, composites and magnetic materials showed remarkable differences in their heating behaviors and microstructural developments. In some cases when exposed to separate fields certain materials were found to have de-crystalized in a matter of few seconds.

11:00 AM Break

11:10 AM Invited

Steel Production with Microwave Assisted Electric Arc Furnace Technology: *Jiann-Yang Hwang*[1]; Xiaodi Huang[1]; Shangzhao Shi[1]; [1]Michigan Technological University

Microwave assisted electric arc furnace technology is a new steelmaking technology under development at Michigan Technological University. This technology is a revolutionary change from the current technology. It is achieved through the combination of microwave, electric arc and exothermal heating. This technology can produce molten steel directly from a shippable agglomerate (green ball) consisting of iron oxide concentrate, coal, and fluxing agent without the intermediate steps of coking, sintering, BF ironmaking, and BOF steelmaking. The unique aspect of this technology utilizes the advantages of rapid volumetric heating, high energy efficiency, and chemical reaction acceleration through the use of microwaves. The viability of the technology lies in the fact that iron ore and carbon are excellent microwave absorbers. This new, simplified process translates into less capital cost, higher productivity, less environmental pollution and treatment cost, higher energy efficiency, and lower production cost.

11:40 AM

Microstructure Prediction and Experiment for Aluminium Alloy 2014 during Hot Ring Rolling Process: *Jian Lan*[1]; Lin Hua[1]; [1]Wuhan University of Technology

Mechanical properties of Al-based Alloy 2014 depend on the grain size, as well as the presence of strengthening phases. The grain size of aluminum alloy parts can be controlled by the thermo-mechanical processes, including heating, forging and cooling sequences. Ring rolling process is usually applied to form seamless ring parts and is a non-steady state throughout. The ring experiences complicated deformation. A series of constitutive equations for dynamic recrystallization, meta-dynamic recrystallization and grain growth were developed and implemented into a 3D finite element simulator, to predict the evolution of grain size in Alloy 2204 ring rolled part. The microstructure and chemical composition of ring part was obtained using SEM, EDS. The microstructure prediction was validated by comparing the simulated grain structure with that of the experimental rolled ring part.

12:05 PM

Study on Microstructure Evolution of Aluminium Alloy 2014 Conical Ring in Hot Rolling: Hua Lin[1]; *Jia Gengwei*[1]; [1]Wuhan University of Technology

A kind of aluminium alloy 2014 conical ring was manufactured through hot ring rolling. In this article, microstructure evolution of aluminium alloy 2014 was studied during hot ring rolling by using SEM, EDS and TEM. The results show that the grain size becomes inhomogeneous after hot ring rolling. Grain size becomes finer and even sub-grains and dislocation cells appear in local region. Coarse grains mostly concentrate in the surface layer and there exist sub-grain structure in inner layer of conical ring. The deformation of various impurity phase has a close relationship with dislocation concentration and formation of micro-cracks. The reason of that is because recrystallization behavior didn't finished completely due to the difference between the speed of hardening and recrystallization of aluminium alloy 2014 during hot ring rolling. Based on the results of microstructure evolution the optimal technological parameters of aluminium alloy 2014 conical ring were determined.

12:30 PM

Study on Fracture of Aluminium Alloy 2014 Conical Ring in Hot Rolling under Different Temperature: Jia Wei[1]; *Hua Lin*[1]; [1]Wuhan Unversity of Technology

In this paper, various kinds fracture of aluminium alloy 2014 conical ring during hot ring rolling under different temperature were observed and compared by using SEM, EDS. Mechanisms of different fracture types were analyzed and the best temperature for hot ring rolling was determined. The results showed that the characteristic of fracture surface is mainly dimple fracture mixed by cleavage fracture in local areas below 490°. This kind of fracture is resulted from inner micro-cracks that have a close relationship with inclusion, forging defects and rolling ring temperature. Fracture surface will transfer into intergranular fracture completely when heating up to 500°. This kind of fracture is result from a lot of impurity phase precipitated at grain boundary, meanwhile overheating structure and many micro-cracks occurred. Based on the results of fracture analysis optimum hot ring rolling temperature of aluminium alloy 2014 is also determined.

Microstructural Processes in Irradiated Materials: Defect Clusters and Fundamental Radiation Effects

Sponsored by: The Minerals, Metals and Materials Society, TMS Structural Materials Division, TMS/ASM: Nuclear Materials Committee
Program Organizers: Charlotte Becquart, University of Lille; Gary Was, University of Michigan; Brian Wirth, University of California

Thursday AM Room: Europe 8
March 1, 2007 Location: Dolphin Hotel

Session Chairs: Ian Robertson, University of Illinois; Yuri Osetsky, Oak Ridge National Laboratory

9:00 AM Invited

Dynamics of Nanometer-Sized Interstitial-Type Dislocation Loops in Iron by In Situ TEM: *Kazuto Arakawa*[1]; Hirotaro Mori[1]; [1]Osaka University

It is believed that one-dimensional high-speed movement of self-interstitial atom (SIA) clusters plays an important role in radiation-induced microstructural evolution in metals and alloys. Recently, extensive classical molecular dynamics calculations have been performed to elucidate the dynamic behaviour of small interstitial-type dislocation loops—agglomerations of SIAs on a habit plane. In contrast, knowledge on the dynamic behaviour of loops obtained by experimental studies still remains insufficient. In this talk, I will describe recent results of our study on the dynamic behavior of loops in high-purity bcc iron upon high-energy electron irradiation and simple heating, by using in situ transmission electron microscopy. The main topics are as follows: (1) processes of motion (prismatic glide and self-climb) of both types of loops (those with the Burgers vectors of 1/2<111> and <100>), (2) processes of interaction between loops.

9:35 AM

TEM Characterization of Defects in Fe: A Simulation Point of View: *Robin Schaeublin*[1]; Amuthan Ramar[1]; Ari Harjunmaa[2]; [1]Centre de Recherches en Physique des Plasmas-Ecole Polytechnique Federale de Lausanne; [2]University of Helsinki

Irradiation of Fe and ferritic-based alloys leads to nanometric defects, such as cavities, secondary phase precipitates and dislocation loops, that generally degrade mechanical properties It is thus of crucial importance to be able to characterize them. Transmission electron microscopy (TEM) remains the method of choice for that purpose. The aim is to investigate by simulation the limits of TEM in the identification and characterization of nanometric defects in Fe. The samples are constructed by molecular dynamic simulations using empirical potentials and the embedded atom method. TEM image simulations are based on the multislice method, thus avoiding the limitation of the column approximation. It appears that indeed there are limitations that impede characterization of nanometric defects but simulations allow designing new methods to overcome these limitations. They will be presented here.

9:55 AM

Vacancy and Vacancy Cluster Properties in bcc Transition Metals Investigated by Density Functional Theory: Charlotte Becquart[1]; *Christophe Domain*[2]; [1]LMPGM, UMR 8517; [2]EDF

The formation and binding energies of vacancy and vacancy clusters in body centered metals (bcc) have been determined by ab initio calculations. The bcc transition metals (V, Cr, Fe, Nb, Mo, Ta and W) are compared. The results indicate that each class of elements behaves differently depending whether they belong to the VB (V, Nb, Ta) or VIB (Cr, Mo, W) column. Among the

transition metals, Fe also strikes out. The vacancy binding energies are larger for VIB and Fe, and to a less extent are increasing from 3d to 5d elements.

10:15 AM

Self-Interstitial Defects in hcp Metals from First Principles: New Structures and Migration Paths: *Guillaume Vérité*[1]; François Willaime[1]; Chu Chun Fu[1]; [1]CEA Saclay

Zirconium alloys, which are widely used in the nuclear industry, have a hexagonal close packed (hcp) structure. The properties of interstitial type defects in these materials are particularly important to understand their microstructural evolution under irradiation. We have performed a systematic study, based on first principles calculations using the SIESTA code, of the structure of self interstitials in pure Zr, and in two other hcp metals, namely Ti and Hf. We have evidenced two new families of low energy and low symmetry configurations. The electronic origins of the discrepancies with empirical potential results for the relative stabilities of these configurations are discussed. The migration paths have been computed in Zr. These new configurations often appear as intermediate states between high symmetry configurations. These results are shown to contribute to reconcile theory with experimental evidences from internal friction and resistivity recovery measurements.

10:35 AM Break

10:50 AM

The Effect of Interface Structure on the Reduction of Radiation Damage in CuNb Multilayers: *Michael Demkowicz*[1]; Richard Hoagland[1]; Amit Misra[1]; Yun-Che Wang[1]; [1]Los Alamos National Laboratory

Simulations of radiation damage cascades near Kurdjumov-Sachs interfaces in CuNb multilayers show that—in agreement with experimental findings—CuNb interfaces remain morphologically stable under 33keV He irradiation. The estimated number of interstitials created in the multilayer structures is half of that observed for bulk FCC Cu and BCC Nb. The origins of reduction in radiation damage are described in terms of the properties of two distinct CuNb interface structures. The behavior of point defects, particularly with respect the to the defect core size, is shown to depend upon the atomic arrangement at the interfaces, influencing the rate of interfacial Frenkel pair recombination. Based on insight gained from CuNb, other pairs of materials that may exhibit radiation damage resistance in a multilayer microstructure are identified. This work was supported by the U.S. DOE Office of Basic Energy Sciences, Division of Materials Sciences and the LANL Directed Research and Development Program.

11:10 AM

Grain Growth in Nanocrystalline Metal Thin Films under In Situ Ion-Beam Irradiation Viewed as a Thermal Spike Phenomenon: Experiment vs. Theory: *Djamel Kaoumi*[1]; A. Motta[1]; R. Birtcher[2]; [1]Pennsylvania State University; [2]Argonne National Laboratory

Grain-growth in nanocrystalline metal thin-films under ion-beam-irradiation was studied experimentally In-Situ in a TEM at temperatures ranging from 20 to 773K. The average grain-size increased monotonically with ion-dose according to:D^n-D^n=KΘ, until it reached a saturation value. Temperature-wise three regimes are observed: (I) a low-temperature ballistic regime where grain-growth kinetics are independent of irradiation-temperature: grain-boundary migration is controlled by intra-cascade ballistic processes,(II) a higher-temperature regime where the kinetics are enhanced by increasing irradiation-temperature: grain-boundary migration is the combined result of irradiation and temperature, (III) a purely thermal regime. The phenomenon is modeled as a thermal-spike phenomenon in which the atomic jumps across grain-boundaries, promoting grain-boundary migration, are induced by the temperature-spikes in the cascades. An expression for grain-boundary mobility is derived which is independent of temperature in the ballistic regime. In the thermally-assisted regime, it is corrected with a temperature-dependent term. The model and the experimental results are compared.

11:30 AM

Molecular Dynamics Simulation of Radiation Damage in Uranium Dioxide: *Taku Watanabe*[1]; Srinivasan Srivilliputhur[2]; Susan Sinnott[1]; Blas Uberuaga[2]; James Tulenko[3]; Robin Grimes[4]; Marius Stan[2]; Stuart Maloy[2]; Simon Phillpot[1]; [1]Department of Materials Science and Engineering, University of Florida; [2]Los Alamos National Laboratory; [3]Department of Nuclear and Radiological Engineering, University of Florida; [4]Department of Materials, Imperial College

Uranium dioxide has been the dominant nuclear reactor fuel material for nuclear power generation for decades. Irradiation causes point defects to form, diffuse, annihilate and aggregate within the crystal. Over extremely short times (order of pico-seconds), collision cascades create damage, most of which quickly anneals. We performed molecular dynamics (MD) simulations to investigate the effects of irradiation on the microstructure of UO_2. We compare two different models for the atomic interactions; the major differences between the two models are the charges of uranium and oxygen atoms and the inclusion of covalency in the short-range interaction. The simulations were performed by imparting a large kinetic energy to a primary knock-on atom (PKA). Effects of PKAs in different low-index crystallographic directions were also investigated. Radiation damage on polycrystalline structures is also demonstrated. This work was funded by DOE-NERI Award DE-FC07-05ID14649.

11:50 AM

A Modified Hard-Sphere Model for the Viscosity of Irradiated U-Si and U-Al Alloys: *Jeffrey Rest*[1]; [1]Argonne National Laboratory

Irradiated U-Si compounds have been observed to go amorphous under irradiation and undergo gas-bubble swelling. Drawing an analogy between the structure of an irradiated amorphous material and that of a liquid, a hard sphere model of binary fluids has been developed and applied to the U-Si and the U-Al systems. This model views each alloy component, before mixing, as a collection of hard spheres of suitable diameter; then, on mixing, the hard sphere diameters are adjusted such that the observable mean volume per atom of the alloy is recovered. The principle difference between a real liquid metal and a hard sphere liquid is provided by the attractive forces of the real particles which gives rise to cohesion of the real liquid. A correction due to such attractive forces is implemented by adding the effect of a uniform negative background potential to the hard sphere model. Results are compared to data.

12:10 PM

Influence of Delta-Phase Metastability on the Radiation Damage Properties of Plutonium-Gallium Alloys: *Steven Valone*[1]; Michael Baskes[1]; Richard Martin[2]; [1]Los Alamos National Laboratory/MST-8; [2]Los Alamos National Laboratory/T-12

Modeling the evolution of plutonium-gallium (Pu-Ga) alloys is extremely important for understanding how these actinide materials age. Aging emanates from spontaneous fission of the Pu resulting in daughter products such as helium (He) and uranium, interstitials, and vacancies. To aid in our understanding, the modified embedded atom method (MEAM) formalism has been applied to the Pu-Ga-He system. The behavior of defects in the fcc phase of Pu-based materials is strongly influenced by the metastability of this phase. The influence of this metastability on minimum displacement threshold energy, point defect characteristics, and He bubbles is delineated. References: M. I. Baskes, Phys. Rev. B 46, 2727 (1992); M. I. Baskes, Mater. Sci. Eng. A261, 165 (1999); S. M. Valone, M. I. Baskes, and R. L. Martin, Phys. Rev. B 73, 214209 (2006) and references therein.

Structural Materials Division Symposium: Mechanical Behavior of Nanostructured Materials, in Honor of Carl Koch: Microstructure and Mechanical Properties of Nanostructured Materials

Sponsored by: The Minerals, Metals and Materials Society, TMS Electronic, Magnetic, and Photonic Materials Division, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Chemistry and Physics of Materials Committee, TMS/ASM: Mechanical Behavior of Materials Committee, TMS: Nanomechanical Materials Behavior Committee

Program Organizers: Xinghang Zhang, Texas A&M University; Yuntian Zhu, Los Alamos National Laboratory; Michael Rigsbee, North Carolina State University; C. Suryanarayana, University of Central Florida; Haiyan Wang, Texas A&M University; C. T. Liu, Oak Ridge National Laboratory

Thursday AM — Room: Asia 5
March 1, 2007 — Location: Dolphin Hotel

Session Chairs: Haiyan Wang, Texas A&M University; Donald Brenner, North Carolina State University

9:00 AM Invited

Deformation-Induced Grain Agglomeration in Nanocrystalline Ni: *Scott Mao*[1]; Zhiwei Shan[1]; Jörg Wiezorek[2]; James Knapp[3]; David Follstaedt[3]; Eric Stach[4]; [1]Mechanical Engineering, University of Pittsburgh; [2]Materials Science and Engineering, University of Pittsburgh; [3]Sandia National Laboratories; [4]School of Materials Engineering, Purdue University

In general, the plastic behavior of crystalline materials is mainly controlled by the nucleation and motion of lattice dislocations. We used in situ dynamic transmission electron microscopy to observe nanocrystalline nickel with an average grain size of about 10 nanometers, which shows deformation-induced grain agglomeration. It has been found that grain boundary mediated processes have become a prominent deformation mode. Additionally, trapped lattice dislocations are observed in individual grains following deformation. This change in the deformation mode arises from the grain-size dependent competition between the deformation controlled by nucleation and motion of dislocations and the deformation controlled by diffusion assisted grain boundary processes. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:20 AM

Plastic Deformation in Nanocrystalline Ni: *Xiao-Lei Wu*[1]; En Ma[2]; [1]Institute of Mechanics, Chinese Academy of Sciences; [2]Johns Hopkins University

A TEM study has been carried out to uncover how twins and dislocations accommodate large plastic strains and accumulate in tiny nanocrystalline Ni grains during low-temperature deformation. We first illustrate four mechanisms of deformation twinning in nanocrystalline Ni and then reveal trapped full dislocations of high density in the grain interior and near the grain boundaries. Dislocations within the grains are in the form of individual dislocations, dislocation loops, and dipoles, with the latter determined as the most proficient. The preferential deformation in the vicinity of grain boundaries and twin boundaries, for dislocation storage and accommodation of large plastic strains decomposing nangrains, will also be discussed.

9:35 AM Invited

Response of Sub-Nanometer Structures in Metallic Glass to Pressure and Stresses: *Evan Ma*[1]; [1]Johns Hopkins University

Among Prof. Koch's many publications, his pioneering paper on deformation-driven amorphization of Ni-Nb is by far the best cited (780 citations as of 2006). Under the high (many GPa) pressure/stresses during ball collisions, severe deformation occurred in the metal mixture, leading to nanostructures and a crystal-to-amorphous transformation. This work opened up a new paradigm in the field of mechanical alloying/milling. It is therefore appropriate to discuss, at this symposium in honor of Prof. Koch, how the internal sub-nanometer scale structures [Nature 439 (2006) 419] evolve under external forces. We will tune the local structure of a metallic glass using hydrostatic pressure [APL 88 (2006) 171906] and introduce the idea of polymorphic amorphous-to-amorphous transformation [to be published]. This will be discussed in light of the visitation of different energy basins in the potential energy landscape, including the plastic flow in an activated process hopping over barriers between nearby basins.

9:55 AM

Microstructure and Properties of Vacuum Hot Pressing SiC/TiCuNiSn Bulk Nanocomposites: *Pee-Yew Lee*[1]; Chia-Chun Wu[1]; [1]National Taiwan Ocean University

In the present study, the preparation of Ti50Cu28Ni15Sn7 metallic glass composite powders was successfully synthesized by the mechanical alloying of powder mixtures of pure Ti, Cu, Ni, Sn and SiC after a 6h milling. In the ball-milled composites, the initial SiC particles were homogeneously dispersed in the Ti-based alloy glassy matrix. The metallic glass composite powders were found to exhibit a large supercooled liquid region before crystallization. Bulk nanocomposite compact discs were obtained by consolidating the 6h as-milled composite powders by vacuum hot pressing process. The microstructure of the Ti50Cu28Ni15Sn7 bulk nanocomposite with 8 vol. % SiC additions exhibited an amorphous/nano matrix embedded with SiC nanoparticles ranging from 20 to 300 nm. A significant hardness increase with the SiC additions can be achieved for the Ti50Cu28Ni15Sn7 bulk nanocomposite. These bulk nanocomposite exhibit good mechanical properties of 1.87~2.12 GPa for compressive strength and 1.86~2.08 for compressive elastic strain.

10:10 AM

Synthesis of High-Density Refractory Metal/Metallic Glass Nano-Composites: *Dan Sordelet*[1]; Min Ha Lee[1]; Ryan Ott[1]; [1]Ames Laboratory

Shear localization of bulk metallic glasses makes them candidates for some specific applications such as kinetic energy penetrators, but densities are in general too low for consideration. One possible solution is to introduce tungsten into a BMG matrix to achieve the required combination of density and deformation behavior. However, the use of body-centered cubic metals to increase the density presents another problem as they are notoriously resistant to shear localization because of their strong strain-rate sensitivity. We have expanded on the recent discovery that certain bcc metals exhibit a decrease in their strain rate sensitivity and show adiabatic shear-localized flow when deformed under uniaxial dynamic compressive loading conditions. Uniformly-layered nanometer-scale tungsten/metallic glass composite particles were fabricated by a milling process and subsequently consolidated by warm extrusion into fully dense rods. Deformation during quasistatic compression tests exhibited highly localized shear flow in these novel tungsten/metallic glass composites.

10:25 AM Break

10:35 AM

Microstructural Defects in Shocked Nanocrystalline Ni: *Hussam Jarmakani*[1]; Eduardo Bringa[2]; Marc Meyers[1]; [1]University of California-San Diego; [2]Lawrence Livermore National Laboratory

This current effort aims at understanding the mechanisms of defect generation in nanocrystalline (nc) Ni deformed at very high strain-rates, larger than 10^6/s. Using the Zerilli-Armstong constitutive description, a model was developed that determines the critical twinning pressure as a function of grain size for shock-deformed Ni. We find a twinning threshold which is consistent with current experiments,[1] and predict a significant lowering of the threshold for Ni alloys with lower stacking fault energy. To understand nc deformation at the atomic scale, we have carried out molecular dynamics (MD) simulations.[2] However, these were simulations of shocks in Cu instead of Ni. We have now carried out similar simulations for Ni, with a interatomic potential that reproduce well the high stacking fault energy of Ni, and discuss how the microstructure changes with respect to the low stacking fault energy case of Cu nc. The work at LLNL was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under contract of No.W-7405-Eng-48, with funding from the Laboratory Directed Research and Development program. [1]APL paper, Wang et al. [2]Science, Bringa et al.

10:50 AM Invited
Atomic-Continuum Simulations of Metal Contacts under High Electro-Magnetic Stress: *Donald Brenner*[1]; [1]North Carolina State University

Metal contacts under high electro-magnetic stress play a key role in technologies that include RF-MEMS switches and electromagnetic launchers. We recently developed a methodology that couples classical molecular dynamics simulations with grid-based numerical solutions to continuum heat and current flow equations. Two sets of simulations using this methodology will be discussed, compression of gold nano-asperities, and asperity-on-flat copper-aluminum interfaces sliding at high velocities and current densities. For the former, the simulations predict formation of nano-wires during unloading that melt via Joule heating at a critical current density. For the copper-aluminum interfaces the simulations predict aluminum transfer onto copper independent of Joule melting, but that Joule melting reduces cold welding and aids in lubrication. Implications for understanding failure of these systems will be discussed.

11:10 AM
Microstructure/Properties Relationship in Nanomaterials: *Alla Sergueeva*[1]; Daniel Branagan[1]; Amiya Mukherjee[1]; [1]University of California

In recent years, properties of technologically attractive nanocrystalline materials have become more prominent in the mainstream scientific community. In this work a review on the current understanding of the effects of microstructural characteristics on properties of nanocrystalline materials produced by different methods is presented. The microstructural information with the experimental data obtained from these nanoscale materials was analyzed in the context of the material response at really diminished length scales. An experimental data arising from testing at different conditions clearly demonstrate that some microstructural features other than just grain size (grain boundary structure, grain size distribution, phase composition, etc.) can also be responsible for the exhibited material behavior. This investigation was supported by NSF grant (NSF-DMR-0240144).

11:25 AM
Mechanical Properties of UFG Iron with Non-Equilibrium and Equilibrium Grain Boundaries: *Julia Ivanisenko*[1]; Kejing Yang[2]; Maxim Murashkin[3]; Askar Kilmametov[3]; Ruslan Valiev[3]; Hans Fecht[2]; [1]Forschungszentrum Karlsruhe; [2]Ulm University; [3]Ufa State Aviation Technical University

Severe plastic deformation (SPD) offers a promising way for producing ultrafine grains (UFG) in metals and alloys, and consequently for enhancement of their strength. Furthermore, SPD-processed materials can demonstrate also significant ductility. However the microstructure of such materials is very complex and typically their grain boundaries (GB) contain high density of extrinsic dislocations leading to non-equilibrium GB structure with increased excess energy and internal stresses. We investigated the tensile properties of UFG iron processed by high pressure torsion in as-processed state and after recovery anneals. Using orientation imaging microscopy we show that anneals in temperature range from 100°C and 450° hadn't led to notable change in a mean grain size and grain misorientations, but internal stresses decreased dramatically, indicating recovery of GBs. As result the mechanical behaviour of UFG iron has been changed. The influence of GB structure on mechanical properties and hardening mechanisms in UFG metals is discussed.

11:40 AM
Experimental Evidences of Transition Behavior in Nanocrystalline Metals: *Hongqi Li*[1]; Hahn Choo[1]; Fereshteh Ebrahimi[2]; Tarik Saleh[3]; Ulrich Lienert[4]; Peter Liaw[1]; Yang Ren[4]; [1]University of Tennessee; [2]University of Florida; [3]Los Alamos National Laboratory; [4]Argonne National Laboratory

It has been accepted that there exists a strongest grain size, i.e. critical grain size, with decreasing the grain size to nanoregime. Both computer simulation and theoretical calculation results show that the deformation mechanisms are different beyond and below this critical point. However, the experimental validation in bulk nanomaterials is lacking and of fundamental interest. Here, we used neutron and synchrotron diffraction sources to characterize the deformation behavior in coarse-grained and nano-grained Ni alloys. The analysis reveals that the microscopic deformation behavior demonstrates a breakdown at the nano-grained scale. In addition, the fractography also exhibits a transition from the conventional void-void dimple feature to the void-cone characteristic as the grain size is reduced below the critical grain size. This work was supported by the National Science Foundation under grant DMR-0231320 at the University of Tennessee with Dr. Huber as the Program Director and DMR-9980213 at the University of Florida.

11:55 AM
Cold Spray Deposition of Nanocrystalline Metals and Composites: *Leonardo Ajdelsztajn*[1]; Bertrand Jodoin[2]; Enrique Lavernia[1]; [1]University of California Davis; [2]University of Ottawa

In this work various metals, alloys and particle reinforced composites were mechanically milled under liquid nitrogen to achieve a nanocrystalline grain size in the range of 20 to 30 nm. The powders were subsequently sprayed using a nozzle designed with a validated numerical model for cold spray technology. The resulting coatings were evaluated using scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD) micro- and nanoindentation. XRD and TEM results show that the nanocrystalline grain structure of the cryomilled feedstock powder was retained after the cold spray process. A significant increase in hardness was observed when comparing the nanocrystalline coating with cast or cold worked conventional material. The ability to use cold spray to produce nanocrystalline large deposits was also demonstrated in this work.

12:10 PM
Functionally Graded Boron-Carbide Nanocomposites for Advanced Armor Applications: *Dustin Hulbert*[1]; Dongtao Jiang[1]; Umberto Anselmi-Tamburini[2]; Amiya Mukherjee[1]; [1]University of California; [2]University of Pavia

Due to its high hardness and low density, Boron Carbide is a very attractive material for armor applications. In this study, we used spark plasma sintering (SPS) to process a functionally graded armor material with functionally graded hardness and toughness. Using SPS, disks of porous boron carbide were created with one surface having a relative density of nearly 95% with the opposing surface having a density of 75%. Pure aluminum was then melt infiltrated into the more porous side at a temperature of 1000°C in a vacuum for at least 1 hour. The resulting material had a nearly linear composition gradient from one surface to another. One side had a hardness and toughness of 2442 kg/mm2 and 5.1 MPam-½ and the other side 1376 kg/mm2 and 6.8 MPam-½ respectively. This material represents a very attractive armor material and showcases the ability of the SPS to produce functionally graded materials.

12:25 PM Concluding Comments by Carl Koch

General Poster Session

Sponsored by: The Minerals, Metals and Materials Society
Program Organizer: James Foley, Los Alamos National Laboratory

Mon PM-Wed PM Room: Northern Hemisphere Foyer
February 26-28, 2007 Location: Dolphin Hotel

Al-Cu Joining: Influence of Various Surface Treatments of Al by Laser: *Vamsi Balla*[1]; Amit Bandyopadhyay[1]; [1]Washington State University

Al-Cu combination is incompatible because they have high affinity to each other at high temperatures and produce brittle, low strength and high electrical resistance intermetallics at the interface during fusion joining. This preliminary work explores the influence of various surface treatments in successfully modifying the Al surface for joining with Cu structures, using laser in Laser Engineered Net Shaping (LENS™). Among the various surface treatments studied, heat treatment at 150°C, 1h resulted in sound interfacial bond between Al and Cu-38wt%Ni coating at 500W laser power – lowest power reported so far for Al laser processing. Other treatments such as anodising and 550°C, 1h before Ni coating revealed excessive intermetallics and large pores at the interface. Finally an attempt has been made to evaluate solderability/brazability of coated Al with Cu structures. It is concluded that by suitably modifying the surface characteristics, the metallurgical compatibility of Al and Cu can be ensured.

Deformation Behavior of 7075 Al Wrought Alloy in the Semi-Solid State: *Young-Ok Yoon*[1]; Shae K. Kim[1]; [1]Korea Institute of Industrial Technology

7075 Al wrought alloy with good mechanical properties has been used with tendency to obtain weight-saving in aerospace, shipbuilding and transport industries. However, it generally allows low extrusion speed and low extrudability index and also causes rather high extrusion pressure when extruded conventionally. Thixoextrusion, one of the thixoforming processes, has advantages of high productivity, reduction of the extrusion pressure, extension of the die life and cost saving due to low energy consumption compared with conventional extrusion processes. Especially, thixoextrusion process is expected to be very effective for hard-to-form materials with high strength. The aim of this study is to investigate the deformation behavior of 7075 Al wrought alloy for thixoextrusion through simple compression test in the semisolid state.

Development of Trivalent Chromium Plating Electrolyte and Plating Process for Automotive Parts: *Beomsuck Han*[1]; [1]Korea Automotive Technology Institute

Every year, end of life vehicles generate between 8 and 9 million tonnes of waste in the Community. The European Commission adopted a Proposal for a Directive which aims at making vehicle dismantling and recycling more environmentally friendly, sets clear quantified targets for reuse, recycling and recovery of vehicles and their components. Hexavalent chromium is a main substance of regulated element.Trivalent chromium baths have numerous environmental and health advantages. We are developing a functional trivalent chromium plating bath using a chromium chloride(CrCl3) as a replacement for commercial hexavalent chromium plating bath. We investigate a functional chromium plating process using a non-toxic trivalent chromium. We compare the chromium coatings fabricated with trivalent chromium plating process with a state of art hexavalent chromium plating process.

Effects of Alumina Additions on Sintering Behavior of $Ce_{0.8}Sm_{0.2}O_{1.9}$ Ceramics Synthesized by Pechini Method: *Joo-Sin Lee*[1]; Kwang-Hoon Choi[1]; Dat Quach[2]; Vladimir Kodash[2]; Joanna Groza[2]; [1]Kyungsung University; [2]University of California

Ceria-based ceramics are difficult to be densified below 1550°C. In order to lower the sintering temperature, other methods such as the use of fine powders and the use of additives should be exploited. The preparation of ultrafine powder has been studied by many investigators. Only limited reports, however, are available on the densification of ceria-based ceramics by using sintering additives. In the present study the effects of alumina additions on the sintering behavior of $Ce_{0.8}Sm_{0.2}O_{1.9}$ ceramics was investigated by the use of powders synthesized by Pechini method. Both sintered density and grain size increased with increasing additive content up to 1 mol% for Al_2O_3 addition. However, they decreased with further addition of the additive. We will discuss the effects of Al_2O_3 additions on the sintering behavior of Sm_2O_3-doped CeO_2, with particular emphasis being placed on the variation in the sintered density and microstructure.

Effects of CaO and Ca on Oxidation and Ignition Resistance of Pure Mg: *Seong-Ho Ha*[1]; Jin Kyu Lee[1]; Hyung-Ho Jo[1]; Shae K. Kim[1]; [1]Korea Institute of Industrial Technology

The applications of Mg alloys are increasing due to their good properties such as low density, good castability and high specific strength. However, molten Mg and Mg alloys are easily ignited and oxidized due to their high reactivity. Many researchers have performed studies to improve ignition and oxidation resistance of Mg through alloying to Mg alloys. It is well known that Ca, though its high cost, is used to improve ignition and oxidation resistance of Mg. However, Ca is difficult to handle due to its high reactivity. It has been attempted to improve ignition resistance of Mg alloys through CaO addition. The aim of this study is to investigate ignition and oxidation behaviors of CaO or Ca added pure Mg. Pure Mg was used instead of Mg alloys to minimize the effects of other elements.

Effects of MgO-Na_2O-P_2O_5 Doping on Flexural Properties of Beta-Tricalcium Phosphate (ß-TCP) Bioceramics: *Robert Fleming*[1]; Samar Kalita[1]; [1]University of Central Florida

Biomedical engineering has been advanced by the discoveries of emerging biomaterials. ß-TCP is an exciting material in this category. The possibility of tailoring its resorption rate, through doping shows promise of using it creating viable controlled strength-loss osteogenic bone-grafts. It has been shown that ß-TCP doped with MgO-Na_2O-P_2O_5, can help control its resorption as well as enhance sintered density by 9%, hardness by 40% and compression strength by 38%. To further explore the benefits of these sintering additives, biaxial flex tests (ASTM F-394) were performed on uniaxially compacted MgO-Na_2O-P_2O_5 doped ß-TCP structures. The results demonstrated as much as a 200% improvement in flexural strength over pure ß-TCP. This is a surprising and fantastic improvement on the flexural strength over pure ß-TCP. XRD analyses, performed on powdered sintered structures, showed no alteration in phase purity. Biodegradation and bioactivity were assessed in simulated body fluid. This presentation will present our findings.

Examination of Thiol Adsorption on Zn-Terminated and O-Terminated ZnO Substrates: *Patrick Sadik*[1]; David Norton[1]; [1]University of Florida

ZnO has been widely studied for a myriad of uses as a transparent semiconductor, as a blue/UV LED, and as a chemical sensor for both gas and liquid phase applications. The ability to grow ZnO high surface area phases including nanowires, nanorods, and nanobelts among other has greatly increased the prospects off achieving single molecule detection. For this reason the adsorption of dodecanethiol on both Zn-terminated and O-terminated ZnO substrates has been examined using RHEED and XPS measurements for temperature increments between 25°C and 500°C. We found that on both Zn-terminated and O-terminated ZnO substrates, dodecanethiol readily adheres to the surface at temperatures in excess of 400°C with the Zn surface having the greater thiol adsorption. On both surfaces the XPS analysis shows that the thiol (-SH) moiety seemed to be largely responsible for surface adsorption.

Fabrication and Reliability Evaluation of Au-Sn Flip Chip Solder Joint: *Jeong-Won Yoon*[1]; Hyun-Suk Chun[1]; Ja-Myeong Koo[1]; Seung-Boo Jung[1]; [1]Sungkyunkwan University

In recent years, the use of optoelectronic packages is increasing rapidly. In these packages, solder alloys are commonly employed for mounting active devices, such as laser diodes, on the substrate of the package. Solders for bonding applications in microelectronic/optoelectronic packages are classified as soft solders and hard solders. Especially, among hard solders, eutectic Au-20wt.% Sn is the preferred alloy because of its relatively low melting point, low elastic modulus, high thermal conductivity, and high strength compared with the other solders. In addition, the flip-chip technology is generally considered the ultimate first level connection because the highest density can be achieved and the path length is shortest so that optimal electrical characteristics are achieved. The objective of this research is to evaluate the interfacial reactions and mechanical reliability of the electroplated Au-Sn flip-chip solder bump. The results on the electroplating, reflowing and bump shear testing will be presented in more detail.

Fabrication of Fe Nanoparticles by Direct Electrochemical Reduction from Fe2O3 Nanoparticles: *Won-Kyu Han*[1]; Jung Ho Baik[1]; So Jin Kim[1]; Chung Man Choi[1]; Sung Goon Kang[1]; [1]Hanyang University

In this report, Fe nano particles have been prepared by direct electrochemical reduction from Fe2O3 nano particles and the reduction mechanism was investigated. To investigate the reduction mechanism, Fe2O3 has been deposited on the AISI 430 by magnetron sputtering in various Ar/O2 ratio and the cyclic voltammetry (CV) was performed in 0.5 M NaCl solution at 300 K. This result indicated that the oxygen from the Fe2O3 was ionized at -1.30 V (versus SCE) and reduced to Fe. The structure of the films were analyzed by XRD, SEM/EDS and XPS.

Laser Surface Modifications of Alumina Ceramic for Applications in Precision Grinding of Materials: *Sandip Harimkar*[1]; Narendra Dahotre[1]; [1]University of Tennessee

Laser Surface modification of the ceramics is a novel technique for achieving improved surface properties. The high cooling rates associated with the laser surface processing results in the formation of various novel phases and morphology. The present study deals with the tailoring the surface morphology of the alumina ceramic with a potential application in micro-scale material removal during surface grinding of materials. Thermal effects during laser surface processing are correlated with subsequent development of the microstructural features such as crystallographic and morphological textures, grain size, depth of melting etc. Also, results of the effects of microstructure development on the grinding performance are presented.

Metal Ion Doped Beta-Tricalcium Phosphate Bioceramic with Improved Properties: *Alton Davenport*[1]; Samar Kalita[1]; [1]University of Central Florida

Recent years have seen a quest for new bioresorbable biomaterials. Beta-tricalcium phosphate (β-TCP) with excellent biocompatibility is ideal for bone-grafting. However, β-TCP suffers from poor flexural strength, poor densification and rapid *in vivo* degradation. In our research, we improved densification and flexural strength of β-TCP by introducing small quantities of divalent metal ions coupled with material-specific sintering which also controlled its degradation rate *in vitro*. High purity metal ions, known to be prevalent in the bone mineral, were introduced into β-TCP powder via ball milling. Dense structures were prepared by uniaxial pressing with green density of 1.7 g/cc and sintered at 1250°C, in air. Results showed 5-12% increase in density, 50-120% increase in microhardness and 30-100% increase in biaxial flexural strength. XRD analysis confirmed no alteration in phase purity. Biodegradation study was performed in dynamic SBF. *In vitro* assay performed, using prostate cancer cells confirmed that these materials were non-toxic.

Microstructural Characteristics and Mechanical Properties of Thixoextruded 2024 Al Wrought Alloy: *Dong-In Jang*[1]; Young-Ok Yoon[1]; Shae K. Kim[1]; Hyung-Ho Jo[1]; [1]Korea Institute of Industrial Technology

The 2024 Al wrought alloy has been used for a wide range of applications such as automobile and aircraft. However, extrusion process for the 2024 Al wrought alloy was not easy due to its low extrudability.Thixoextrusion, one of the thixoforming processes, has advantages of high productivity, reduction of the extrusion pressure and cost saving due to low energy consumption compared with conventional extrusion processes. Especially, thixoextrusion process was expected to be very effective for hard-to-form materials with high strength. In this paper, effects of extrusion parameter, such as extrusion temperature, speed and die bearing length, on the microstructure and mechanical properties of 2024 Al wrought alloy were interested. The thixoextrusion was carried out at 607' and 631' with extrusion speeds of 10'/sec, 20'/sec and 30'/sec. The die bearing lengths were 7' and 15'. The results of thixoextrusion experiments were compared with conventional extrusion results.

Microstructural Evolution of 7075 Al Wrought Alloy for Thixoextrusion Process: *Young-Ok Yoon*[1]; Dong-In Jang[1]; Shae K. Kim[1]; Hyung-Ho Jo[1]; [1]Korea Institute of Industrial Technology

The study for thixoextrusion of 7075 Al wrought alloy was carried out with respect to reheating rate, isothermal holding temperature and time with an emphasis to the effect of homogenization on thixotropic microstructures during the partial remelting. The main emphasis of this study was to investigate feasibility of microstructural control in the low liquid fraction (fL<0.3) for the thixoextrusion of 7075 Al wrought alloy without additional pretreatment. The results show that the liquid fraction and average grain size were almost uniform with respect to isothermal holding temperature and time. It is considered very useful for thixoextrusion in terms of process control such as billet temperature control and actual extrusion time. Microstructural control of 7075 Al wrought alloy both before and after homogenization could be possible and thixotropic microstructures were obtained in both specimens.

Notch Toughness of a Cu-Based Bulk Metallic Glass: *Matthew Freels*[1]; Peter Liaw[1]; Gongyao Wang[1]; [1]University of Tennessee, Knoxville

Cu-based bulk-metallic glasses (BMGs) have received much interest of late due to their high strength and low cost compared to the widely studied Zr-based BMGs. Consequently, it is important that Cu-based BMG systems be further studied and developed. In this study, the fracture toughness of (Cu60Zr30Ti10)99Sn1 BMG was examined using the three-point bending method. Notch toughness tests were performed on an MTS servohydraulic testing machine under constant displacement rates ranging from .1mm/min. Notch radii ranged from 150 μm to 300 μm. Notch depth was kept constant at .45W (2.15 mm). Load versus displacement was monitored during testing. Preliminary results indicate notch toughness values calculated from the maximum load at fracture range from 35 MPa√m up to 65Mpa√m. Fracture surface characteristics, as well reasons for the large variability in the data will be explored.

On the Phase Diagram and Thermodynamics of the Al-Nd-Ni System: A Combined Approach of Experiments, CALPHAD and First-Principles Calculations: *Michael Gao*[1]; Michael Widom[1]; Gary Shiflet[2]; Marek Mihalkovic[1]; [1]Carnegie Mellon University; [2]University of Virginia

A novel approach that combines critical experiments, CALPHAD modeling and first principles (FP) calculations is used to study the Al-Nd-Ni ternary phase diagram and the underlying thermodynamics. Two new ternary compounds are experimentally identified, i.e. Al19Nd3Ni5 and Al5NdNi2. Based on our FP calculations, they are suggested to be isostructural with Al19Gd3Ni5 (Pearson symbol oC108) and Al5CeNi2 (oI16) respectively. Other compounds that are likely stable include Al4NdNi, Al3NdNi2, Al2NdNi, AlNdNi, AlNd2Ni2 and AlNd3Ni8, whose crystal structures are suggested with FP calculations. Several compounds exhibit compositional homogeneity range via Al/Ni substitution that are measured experimentally at 773 K: Al2Nd (~3 at% Ni); Al3NdNi2 (46-52 at% Al); Al5NdNi2 (25-28 at% Al). Based on the present experimental data and FP calculations, the complete phase diagram and the thermodynamic descriptions are determined via CALPHAD modeling. Application to glass formation is discussed in light of present study.

Phase Equilibria Study and Thermodynamic Assessment of the Al-Ce-Co System Assisted by First-Principles Energy Calculations: *Michael Gao*[1]; Necip Unlu[2]; Marek Mihalkovic[1]; Michael Widom[1]; Gary Shiflet[2]; [1]Carnegie Mellon University; [2]University of Virginia

This study investigates the phase equilibria of the Al-rich Al-Ce-Co system using a range of experimental techniques including melt spinning, TEM, EPMA, XRD and DTA. The glass formation range in the Al-rich corner is determined, and a partial 773 K isotherm is constructed. Three stable ternary phases are confirmed, namely, Al8CeCo2, Al4CeCo and AlCeCo, while a metastable phase, Al5CeCo2, was discovered. Also confirmed are our previous results [Metall. Mater. Trans. A 2005;36A:3269.] that a polymorphous transformation of α/βAl3Ce exists in the Al-Ce binary system, and that the transformation between Al11Ce3.oI28 and Al4Ce.tI10 can't be polymorphous. The equilibrium and metastable phases identified by the present and earlier reported experiments are further studied by first-principles calculations. Based on new experimental data and FP calculations, the thermodynamics of the Al-Co-Ce system is optimized using the CALPHAD method. Model calculated phase equilibria and phase boundaries conform with the present experimental results.

Porous Titanium Electrodes for Microbial Fuel Cell (MFC) Applications: David Beeler[1]; Leroy Long[1]; Emily Henderson[1]; Daniel Young[1]; *Raghavan Srinivasan*[1]; [1]Wright State University

Microbial fuel cells (MFC) work on the principle that during metabolism certain bacteria produce electrons which can be harnessed as a source of electrical energy. This paper presents the results of a study on the production and use of porous titanium electrodes in MFC. Electrodes were produced by powder metallurgy (PM) techniques using 20 micrometer CP titanium powder,

and powders of another material as place holders. Mixtures with different titanium to place holder material ratios were cold compacted use to produce green bodies from which the place holder material was etched out. The porous compact was then sintered to produce electrodes for the MFC. Results to be presented include characterization of the titanium electrodes in terms of microstructure, specific surface area, and permeability. Results from the use of the electrodes in MFC will also be presented.

Reaction of Co Phase in the WC-Co Coatings with Molten Zinc: Byeog-Geun Seong[1]; Sung-Hee Kwon[2]; Kyoo-Young Kim[3]; *Kee-Ahn Lee*[2]; [1]Research Institute Science and Technology; [2]Andong National University; [3]POSTECH

The main objective of this study is to investigate the detailed reaction mechanism of Co phase with molten zinc. Pure Co, Co-W alloys specimens were used to understand role of the phase and alloying effect. These specimens were immersion tested in Zn bath. After immersion of Co in a pure molten zinc bath at 460°C to 520°C four kinds of Co-Zn intermetallic compound layers, β1, γ, γ1, and γ2 were formed on the Co matrix. Rate controlling step for this reaction was diffusion through β1 compound layer and the activation energy was calculated to be 214.9 kJ/mole. Co-10%W alloy showed no W alloying effect on the reaction rate in a molten zinc bath but the reaction rates increased as W contents increase to 20% and 30%. β1 layer was not formed on Co-20%W alloy and no stable Co-Zn intermetallic compound layer was found on the Co-30% alloy.

Recovery of Pd(II) and Pt(IV) Ions by Introducing SCN^- Soft Ligand with Tannin Gel: *Yoshio Nakano*[1]; Yeon Ho Kim[1]; [1]Tokyo Institute of Technology

We have developed a new Pd(II) and Pt(IV) recovery process from wastes such as spent catalysts or scraps, which is simple and generates little secondary waste, using tannin gel particles synthesized from condensed-tannin, ubiquitous and inexpensive natural material. We have reported that in chloride solution, Pd(II) ionic species are adsorbed onto the tannin gel particles through inner-sphere redox reaction mechanism: two-electron transfer from tannin gel to chloro-palladium(II) complexes, accompanied by ligand substitution between chloro-palladium(II) complexes and hydroxyl groups of tannin gel. In the present investigation, The intermediate step (ligand substitution) plays an essential role in the Pd(II) and Pt(IV) adsorption, because the ligand substitution rate is increased by introducing a soft ligand (SCN^-). Addition of SCN^- ion to chloride solution leads to the formation of chlorothiocyanocomplexes which is more favourable for the ligand substitution with tannin gel than chlorocomplexes because of the trans-effect.

Reprocessing of Silicon Carbide-Based Inert Matrix Fuels: *Soraya Benitez*[1]; Ronald Baney[1]; James Tulenko[1]; [1]University of Florida

Silicon carbide (SiC) is one of the prime candidates for the fabrication of ceramic based inert matrix fuels (IMF) for the burning of plutonium and for the transmutation of long-lived actinides. However, reprocessing of SiC-based IMF to separate transuranic species for both spent and unspent nuclear fuel from the SiC matrix is not well defined. A potential reprocessing method under investigation is the use of alkali and alkali earth molten salt baths to dissolve the SiC matrix. SiC samples with and without ceria will be reprocessed using the molten salt method to determinate ease of separation, dissolution rates, and resulting compounds. Ceria is used as a surrogate for plutonium and for the transuranic species.

Stress Rupture Property of Inconel 718 Alloy: *Ji Soo Kim*[1]; Chong Soo Lee[1]; [1]Pohang University of Science and Technology

Stress rupture properties of base metal and weldment of Inconel 718 Alloy for aerospace applications were examined in the present study. The specimens were solution heat treated according to the specification of ASM 5596, i.e., heating to a temperature of 980°C, holding at the temperature for an hour and air cooled. Afterward, precipitation heat treatment was done by heating to 720°C for 8 hours, furnace cooled to 621°C, holding at 621°C for 8 hours and furnace cooled. The test temperatures were varied from 649°C to 760°C. With the increase of test temperature, stress rupture life was shortened at the same stress ratio. The weldement was more fragile than the base metal. Detailed microstructures and fracture surfaces after the rupture test were investigated by the optical microscope and SEM.

Study of Hot Deformation Behavior of Ti-6Al-4V Alloy with Widmanstätten Microstructure by Artificial Neural Networks: N. Reddy[1]; *Chan Hee Park*[1]; [1]Pohang University of Science and Technology

The present work demonstrates the use of an artificial neural networks (ANN) model in generating processing maps for hot working processes for Ti-6Al-4V alloy with widmanstätten microstructure. The flow stress data for ANN model training was obtained from continuous compression tests performed on a thermo-mechanical simulator over a wide range of temperatures (700-1100°C) with the strain rates of 0.0001-100 s-1 and true strains of 0.1 to 0.6. It has been found that the flow stress values predicted by the ANN model agree closely with actual experimental values, thus indicating the possibility of using neural networks approach to tackle hot deformation problems. The specimen failures at various instances have been predicted and metallurgical explanations had been presented. The flow stress predicted at finer intervals of temperature and strain rate regions and subsequently processing maps were developed. The safe domains of hot working of alloy were identified and validated through microstructural investigations.

The Effect of Composition of Carbon Fibre on the Mechanical and Morphological Properties of PA6/Carbon Composite: *Albert Ude*[1]; Husna Azhari[1]; [1]National University of Malaysia Bangi

A study to investigate the mechanical property-morphology relationship of polyamide 6 reinforced carbon fibre composites has been carried out. The composites were prepared by melt mixing, in a composition of wt% PA6/wt%CF; 95/5, 90/10, 85/15, 80/20 respectively. The length of the fibre was 500µm. The mechanical properties were measured. These properties were correlated to the morphology. The mechanical properties suggest that carbon fiber has the potentials to reinforce polyamide 6; hence an increase in strength recorded, displaying that strength is a function of the volume of the reinforcement (fibre).Morphological study of the tensile fractured surface showed the mechanism of failure to be the dispersed domain pulling out of a continuous matrix, leaving voids in their alert. The size of the voids seems to correspond with the size of the fibrils, making the inference that the voids observed were space left by the pulled-out fibre distributed in different direction apparently reasonable.

X-Ray Absorption near Edge Structure Analysis of Chromium Oxynitride Thin Films: *Jun Inoue*[1]; Tadachika Nakayama[1]; Tsuneo Suzuki[1]; Hisayuki Suematsu[1]; Weihua Jiang[1]; Koichi Niihara[1]; [1]Nagaoka University of Technology

We have already reported the hardening in Cr(N,O) thin films by the increase in the oxygen content (x). X-ray absorption near edge structure (XANES) in the thin films was observed to clarify electronic structure change associated with the hardening. The Cr(N,O) thin films were prepared by PLD method. The beam line BL-12C of PF in High Energy Accelerator Research Organization was used for XANES measurements. It was found that the ionicity between metal and nonmetal atoms has increased by replacing nitrogen atoms in CrN by oxygen atoms, since the Cr-K edge peak shift to higher energy was observed with increasing x. Furthermore, the peak attributed to the electronic transition from 1s to band that formed by 3deg of metal atom and 2p of nonmetal atoms decreased with x increases. It can be understood the reason for this result is that the total valence electron density increased gradually with increasing x.

***In-Situ* Chemical Oxidation of Soil Contaminated by Benzene, Lead and Cadmium**: Marcia Bragato[1]; *Jorge Tenorio*[1]; [1]Escola Politecnica-Universidade de Sao Paulo

Soil contamination by oil and its derivatives is found at many sites in Sao Paulo, Brazil. In this research, the chemical oxidation was used as remediation method for soil contaminated simultaneously by benzene, lead and cadmium simulating in-situ conditions. Tests were carried out under laboratory conditions. In the oxidation tests the efficiency of Fenton's reagent (H_2O_2/Fe^{+2}) on the benzene oxidation was performed. Under the imposed oxidizing conditions lead in the lecheate increased in TLCP tests. Using the Fenton's reagent the increase of lead concentration in the lecheate was 4 times greater under natural conditions. On the other hand, cadmium presented the opposite behavior, *e.g.*, Cadmium concentration in the lecheate was decreased 50% for the oxidizing conditions.

Development and Validation of High Performance Thick Thermal Barrier Coating (TBC) for Application on Turbine Components: *Gabriele Rizzi*[1]; A. Scrivani[1]; [1]Turbocoating

This paper addresses the development of thick TBC (with thickness in the range of 1.5 - 2 mm), focusing attention on the microstructure and the porosity of the Yttria Partially Stabilised Zirconia (YPSZ) coating, in relation to its resistance to thermal cycling fatigue (TCF). TBC coatings have been produced by means of a NiCoCrAlY bond coat and Yttria Partially Stabilised Zirconia top coat, both sprayed by Air Plasma Spray. The obtained samples have been characterized from the metallographic point of view in order to determine the structure and the porosity of the coating. Finally the samples have been submitted to TCF test, according to the procedure of two important OEMs. The study enabled determination of a good microstructure of the TBC coating with high TCF resistance independent of the porosity of the coating itself.

Development of CVD Overaluminising Method on Different Conicraly Bond Coats Deposited by Low Pressure Plasma Spray (LPPS), High Velocity Oxygen Fuel (HVOF) and Air Plasma Spray (APS): *Gabriele Rizzi*[1]; A. Scrivani[1]; [1]Turbocoating

This paper addresses the study of Aluminium coatings deposited by CVD on CoNiCrAlY bond coats deposited by three thermal spray techniques. The different CoNiCrAlY coatings structure obtained by these three techniques (Low Pressure Plasma Spray or Vacuum Plasma Spray, High Velocity Oxygen Fuel and Air Plasma Spray) with different content of oxides and porosity could affect the deposition rate and quality of the Al coatings. The obtained samples have been characterized from the metallographic point of view (porosity, thickness and structure). Al coating thickness has been taken as parameter in order to define the Al coating deposition rate on the three different CoNiCrAlY coatings. Oxidation test has been performed in order to evaluate and compare the oxidation resistance of this three different coatings.

Self-Organized Periodic Array of Single Crystal Oxide Nano Islands: *L. Zimmerman*[1]; Michael Rauscher[1]; S. Dregia[1]; J. Lee[1]; S. Akbar[1]; [1]Ohio State University

We have deposited a gadolinium doped ceria thin film on an yttria-stabilized zirconia substrate using RF magnetron sputtering. Subsequent spalling of the thin film and a high temperature anneal combine to create a periodic array of single crystal islands with regular size, shape, and distance from their nearest neighbors. The features can be used as a template to transfer the pattern to other materials of interest, with the high strength of the material allowing for superior durability and fidelity of pattern transfer. In its current form, the nanostructure may find use in manipulation of single proteins and single molecules of DNA, as well as in nanoscale analytics. We predict the ability to establish long-range periodicity in the alignment of the islands creating a regular 2D network of nanochannels. These structures represent a tunable, self-assembling, low-cost, non-cleanroom means of producing nanoscale features suitable for nanofluidic channel fabrication and numerous other applications. In this work, we discuss the conditions necessary to create the novel nanostructure, and highlight the influence of annealing on the structure features. We have performed preliminary characterization of the system to determine its intrinsic usefulness for a range of optical, electronic, magnetic, and biological nanofluidic applications. We also discuss early efforts to create nanofluidic devices based on the pattern.

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