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6th Global Innovations Symposium: Trends in Materials and Manufacturing Technologies for Transportation Industries: Bulk Metal Processing

Sponsored by: Materials Processing and Manufacturing Division, MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS), MPMD-Nanomechanical Materials Behavior, MPMD-Phase Transformation Committee-(Jt. ASM-MSCTS), MPMD-Powder Materials Committee, MPMD-Shaping and Forming Committee, MPMD-Solidification Committee, MPMD-Surface Engineering Committee, MPMD/EPD-Process Modeling Analysis & Control Committee

Program Organizers: Thomas R. Bieler, Michigan State University, Department of Chemical Engineering and Materials Science, East Lansing, MI 48824-1226 USA; John E. Carsley, General Motors Corp, Warren, MI USA; Hamish L. Fraser, Ohio State University, Department of Materials Science and Engineering, Columbus, OH 43210-1179 USA; John E. Smugeresky, Sandia National Laboratories, Department 8724, Livermore, CA 94551-0969 USA

Thursday AM Room: 2009
February 17, 2005 Location: Moscone West Convention Center

Session Chairs: Thomas R. Bieler, Michigan State University, Dept. of Cheml. Engrg. & Matls., E. Lansing, MI 48824 USA; Ibrahim Karaman, Texas A&M University, Dept. Mechl. Engrg., College Sta., TX 77843 USA

8:30 AM
Microstructural Engineering of Structural and Smart Materials Using Severe Plastic Deformation for Transportation Industry: G. Guven Yapici[1]; *Ibrahim Karaman*[1]; [1]Texas A&M University, Dept. of Mechl. Engrg., MS 3123, College Sta., TX 77843 USA

This talk will summarize our recent work on severe plastic deformation processing of several structural and smart materials using Equal Channel Angular Extrusion (ECAE). ECAE was achieved by extruding bulk materials through two channels of equal cross section intersecting at an angle of 90° achieving a simple shear deformation in a thin layer at the crossing plane of the channels. We will present the means of engineering of microstructure for high strength and ductility using severe plastic deformation in difficult to work materials such as Ti-6Al-4V, AISI 316L stainless steel and NiTi shape memory alloys and challenges and opportunities for transportation industry. The selected mechanical properties and microstructure will be exhibited. Ti-6Al-4V extrusions revealed that decreasing extrusion temperature and increasing number of passes decreases α plate size and grain size, leading to significant increase in tensile and compressive flow stresses at room temperature. Significant deformation twinning activity was observed for the first time in Ti-6Al-4V and 316L stainless steel at temperatures as high as 800°C (0.65 Tm!). ECAE of NiTi led to the observation of highly organized, twin-related nanograins in the high temperature phase which enhance cyclic stability and fatigue resistance of this alloy. The formation of well-organized twin-related nanograins via severe plastic deformation opens a new opportunity for twinning induced grain boundary engineering in B2 NiTi intermetallics. ECAE is applicable to numerous materials critical to industries ranging from aerospace to automobile and railroad. Therefore, it is of paramount importance to gain control over this processing method for producing desired end microstructures and mechanical properties in favor of transportation industry.

8:50 AM
Semisolid Microstructures of ECAP-Processed Al-9mass%Si-3mass%Cu Alloy: *Yuanwei Song*[1]; Yoshinori Nishida[1]; Teiichi Ando[1]; [1]Northeastern University, Mechl. & Industl. Engrg., 360 Huntington Ave., 334 Snell Engrg., Boston, MA 02115 USA

Effects of equal-channel-angular-pressing (ECAP) on the evolution of semisolid microstructures in an Al-9mass%Si-3mass%Cu alloy were investigated. ECAP-processed specimens held at the eutectic temperature (572¢X C) and semisolid temperatures for various holding times and quenched into water were examined. All of the specimens showed a microstructure indicative of formation of semisolid microstructures consisting of spheriodized ?Ñ grains fully separated by the liquid. The solid fraction of ECAP-processed specimens at the eutectic and semisolid temperatures stayed much higher than the low ?Ñ fractions expected for the ?Ñ ¡V liquid equilibrium in the alloy. Prior processing by ECAP refines the Si particles and homogenizes the cored ?Ñ matrix in the alloy, which helps to retard the formation of liquid. The sluggish liquid formation assures ample time for semisolid forming, providing a workable window for bulk-stock semisolid part forming with near eutectic aluminum die-casting alloys.

9:10 AM
Thermo-Mechanical Processing of a Cast 7XXX Al Alloy Modified with Sc: *Radhakrishna B. Bhat*[1]; Sesh Tamirisa[2]; Oleg N. Senkov[1]; [1]UES, Inc., Matls. & Processes, 4401 Dayton-Xenia Rd., Dayton, OH 45431 USA; [2]Ohio University, Mechl. Engrg., Athens, OH 45701 USA

Al alloys modified with Sc offer significant enhancements in mechanical properties and are attracting attention for aerospace applications. Thermo-mechanical processing (TMP) is an important step in the shape-forming of these alloys to obtain desired shape, microstructure, and mechanical property combinations. The Sc addition is expected to affect the TMP response of Al alloys and a thorough understanding would help in the design and optimization of the process sequences. In this paper, we describe the TMP response of an advanced Sc-modified 7XXX Al alloy produced via direct chill continuous casting. Hot compression tests were conducted in the temperature range of 250 - 500°C and strain rate range of 3´10-4 - 10 s-1. A processing map for hot working is generated based on the analyses of temperature and strain rate sensitivity of the flow stress over the above ranges. Hot deformation mechanisms are identified and correlated with microstructural analysis and hot tensile behavior. The influence of Sc on the hot workability of the alloy is established, and the optimum parameters for TMP will be discussed.

9:30 AM
Microstructure and Tensile Properties of Developmental Al-Zn-Mg-Cu Cast Alloys Modified with Sc and Zr: *Svetlana V. Senkova*[1]; Radhakrishna B. Bhat[1]; Oleg N. Senkov[1]; [1]UES, Inc., Matls. & Processes Div., 4401 Dayton-Xenia Rd., Dayton, OH 45432 USA

The effect of combined addition of Sc and Zr on the microstructure and tensile properties of the direct chill (DC) cast ingots of developmental Al-Zn-Mg-Cu alloys has been evaluated in this work. The properties in both the longitudinal and transverse directions of the cast ingots were determined in as-cast and heat-treated conditions, at room and cryogenic temperatures. Homogenization, solution treatment and aging schedules were optimized to obtain superior mechanical properties. In particular, the Sc-containing developmental cast alloys showed the tensile properties, which are much better than the properties of any commercial cast Al alloys and are similar to the properties of a wrought 7075-T6 alloy. The strengthening mechanism, optimum content of the dispersoid-forming elements, and the processing parameters responsible for these improvements are discussed.

9:50 AM
Effect of Crystallographic Texture on Tensile Properties of a 7XXX Alloy with Sc Addition: *Oleg N. Senkov*[1]; Svetlana V. Senkova[1]; Radhakrishna B. Bhat[1]; [1]UES, Inc., Matls. & Processes Div., 4401 Dayton-Xenia Rd., Dayton, OH 45432 USA

Room temperature tensile properties of a 7XXX series alloy containing 0.18% Sc were studied after high-temperature extrusion and forging followed by heat treatment. The extruded alloy showed superior tensile strength (UTS=730 MPa) and ductility (El=15%) in the longitudinal direction; however, the properties in this direction reduced considerably, to 630 MPa and 8%, respectively, when forging was applied in the direction opposite to extrusion. Orientation image microscopy (OIM) analysis was conducted to understand why the properties of the extruded product degrade after forging. It was found that the main processes responsible for such behavior are the dynamic recrystallization occurring during forging and leading to grain coarsening and change in the crystallographic texture. The decrease in the tensile strength directly correlates with a decrease in the Taylor factor and the decrease in ductility can be related to large differences in the Schmidt factor of neighboring grains in the forged material.

10:10 AM Break

10:25 AM
Age-Hardening and Plastic Anisotropy in Extruded AA6xxx and AA7xxx Profiles: *Hans Bjerkaas*[1]; Snorre Kjørstad Fjeldbo[1]; Hans Jørgen Roven[1]; Jarle Hjelen[1]; Trond Furu[2]; [1]Norwegian University of Science and Technology, Dept. of Matls. Tech., Trondheim N-7491

Norway; [2]Hydro Aluminium R&D Materials Technology, Sunndalsøra N-6600 Norway

To understand plastic anisotropy in extruded aluminium profiles and how this anisotropy changes during precipitation is essential in order to control forming of aluminium profiles. Several authors have reported large changes in the plastic anisotropy as a function of precipitation in textured alloys. However, the predicted anisotropy deviates from the observed anisotropy when coherent and semi-coherent precipitates are introduced to the microstructure, indicating that such precipitates strongly affects the deformation process. In the present work alloys from the AA6xxx and AA7xxx systems are studied and compared. The extruded profiles investigated have a strong texture, giving rise to a substantial plastic anisotropy in the solution treated condition. Both the effects of natural and artificial ageing are studied. The observed plastic anisotropy is compared with predictions from the Taylor/Bishop/Hill model based on input from orientation data obtained by microdiffraction in a FE-SEM.

10:45 AM

Further Developments in the Precision Forging Technology for High Duty Automotive Parts: Bernd-Arno Behrens[1]; Steffen Reinsch[1]; Axel Specker[1]; *Kathrin Telkamp*[1]; [1]IPH-Institut für Integrierte Produktion Hannover gGmbH, Process Tech., Hollerithallee 6, Hannover 30419 Germany

Precision forging is defined as a flashless forging operation, which generates high quality parts by means of surface quality and accuracy to dimension. So far precision forging processes have been designed for connecting rods, gears and hand tools. The diversification of this group of parts with the design of a precision forging process for crankshafts not only expands the applicable product range but also requires new technical solutions. The most obvious differences between currently produced precision forged parts and crankshafts are the bigger mass of the crankshaft and the extremely asymmetric mass distribution. To meet this challenge a new forging chain with three forming processes was developed. Finite-element-programs have been used for the verification of the applicability definition of the process limits. Practical testing of the processes showed the feasibility of forging crankshafts with flashless precision forging technology and gave references for the verification of the processes.

11:05 AM

Effects of Working, Heat Treatment, and Aging on Microstructural Evolution, Phases, and Crystallographic Texture in Ti-6Al-4V Wire: Liang Zeng[1]; *Thomas R. Bieler*[1]; [1]Michigan State University, Cheml. Engrg. & Matls. Sci., E. Lansing, MI 48824-1226 USA

Crystallographic texture and microstructure was measured on Ti-6Al-4V wire in as-received, cold extruded, heat treated in the alpha+beta phase field, water quenched, and aged samples. Extrusion strengthened the as-received prism fiber texture, but after solutionization and quenching, a secondary basal fiber texture emerged, indicating that a strongly preferred variant selection occurred during quenching. The selection of preferred variants in the alpha-beta-alpha transformation cycles is discussed in relation to shears imposed in the beta phase due to differential thermal expansion between misoriented a regions. After artificial aging, alpha' and beta phases were present, but subsequent natural aging for a year led to elimination of alpha" and a reduction in the amount of the beta phase. The effect of extrusion and solutionization time on the orientations of alpha, alpha', alpha", and beta phases are discussed in the context of the known physical metallurgy of titanium alloys.

11:25 AM

Effect of Oxygen Content on Fatigue Properties of Single-Melt PAM Processed Forged Ti-6Al-4V Bell Housings for Lightweight 155mm Howitzer: *Mustafa Guclu*[1]; Ibrahim Ucok[1]; Hao Dong[1]; Chris Hatch[2]; [1]Concurrent Technologies Corporation, 100 CTC Dr., Johnstown, PA 15904 USA; [2]U.S. Army ARDEC, Bldg. 151, Picatinny Arsenal, NJ 07806 USA

Ti-6Al-4V (Ti-6-4) is the main structural alloy for the new lightweight 155mm Howitzer (LW155) and was selected for reduced weight and enhanced performance. However, Ti-6-4's relatively high cost compared to steel and aluminum alloys has limited its usage in other non-aerospace applications. It is clear that, in the near term, the use of single-melt (SM), high oxygen titanium alloys such as those made by plasma arc melt (PAM) processing is at the forefront of low-cost titanium alloys. In this study, Ti-6-4 bell housings for the Lightweight 155mm Howitzer were manufactured by forging using low-cost SM PAM billet stock at three oxygen levels, 0.16, 0.20 and 0.24 wt%, along with a standard double vacuum arc remelted (2XVAR) billet stock at 0.17 wt% oxygen for baseline comparison. To demonstrate the viability of SM PAM material, mechanical properties of mill-annealed forgings were characterized by microstructure, tensile and smooth bar axial fatigue testing. SM PAM forgings met mechanical property requirements of ASTM B381 and AMS 4928 specifications, and exhibited higher tensile and yield strengths than 2XVAR material. Tensile and yield strengths increased with increasing oxygen content with a gradual reduction in ductility values. All SM PAM forgings exhibited slightly higher fatigue strengths compared to those of 2XVAR in the longitudinal orientation. Microstructures of all forgings were similar to those of conventional a-b forgings. The total a content in SM PAM forgings increased with increasing oxygen content. Based on the testing and characterization results, forgings made using SM PAM material up to 0.24 wt% oxygen are viable for bell housing application. The data presented in this paper can be useful to designers in their efforts to introduce low-cost SM PAM Ti-6-4 alloy forgings into various U.S. defense applications. This work was conducted by the National Center for Excellence in Metalworking Technology, operated by Concurrent Technologies Corporation under Contract No. N00014-00-C-0544 to the Office of Naval Research as part of the U.S. Navy Manufacturing Technology (ManTech) Program.

11:45 AM

Texture and Microstructure Development in Ti-10-2-3: *Seema L. Raghunathan*[1]; Martin Jackson[1]; Richard J. Dashwood[1]; David Dye[1]; [1]Imperial College, Dept. of Matls., Royal Sch. of Mines, Prince Consort Rd., London SW7 2BP UK

Ti-10V-2Fe-3Al (Ti-10-2-3) is a high-strength, high-toughness, deep-hardenable, near-beta titanium alloy widely used for near-net shape forging. It has become clear that the microstructure and resulting properties of most near-beta alloys are very sensitive to the forming variables, even during isothermal forging, and this has, to date, required empirical optimization. The cost associated with this approach is a significant driver for the development of models capable a predicting the final textures and microstructures that result. This work, which is based on an earlier microstructural study, aims to examine the effect of the forming variables on texture development. Neutron diffraction and EBSD results for the misorientation and macroscopic textures are presented, and an attempt is made to rationalize them with the aid of a finite element model of the strain path and a sequentially coupled visco-plastic self-consistent (VPSC) model of deformation that excludes the effects of recrystallization.

Alumina and Bauxite: Alumina Quality

Sponsored by: Light Metals Division, LMD-Aluminum Committee
Program Organizers: Dag Olsen, Hydro Aluminium AS, Porsgrunn 3907 Norway; Travis Galloway, Century Aluminum, Hawesville, KY 42348 USA; Halvor Kvande, Norsk Hydro ASA, Oslo N-0240 Norway

Thursday AM — Room: 2005
February 17, 2005 — Location: Moscone West Convention Center

Session Chair: Carl Behrens, Hydro Aluminium, Alumina & Bauxite, Porsgrunn N-3907 Norway

8:30 AM

Alumina Quality Improvements at the Alpart Refinery, Nain, St Elizabeth, Ja.: *Patrick Donovan James*[1]; [1]Alumina Partners of Jamaica, Techl., PO Box 529, Arabi, LA 70032 USA

In a quest to be named among the preferred Alumina suppliers in the world market, Alumina Partners of Jamaica (Alpart) embarked on a stepwise program over the past few years to demonstrate significant improvement in its product quality. The area of focus has surrounded particle size, particle strength and dustiness. The approach involved structural, procedural and technological changes which are a blend of known practices worldwide. This paper describes the approach taken, the step changes taken to date, the pitfalls along the way as learning for the future and results achieved.

8:55 AM

Effect of the Total Soda on the CMR of the Agglomeration Zone and Occluded Soda in the Precipitation Circuit at CVG Bauxilum: *Jesús Alcalá*[1]; Nelson Angulo[1]; [1]CVG Bauxilum Alumina Plant, Av. Fuerzas Armadas, Zona Industl. Matanzas, Ciudad Guayana, Edo. Bolívar Venezuela

The occluded soda is one of the main quality characteristic of metallurgic grade calcined alumina and the CMR in the agglomeration zone of the precipitation circuit defines the productivity behavior throughout the system, these two parameters are related with the

levels of impurities and other variables of the process. At CVG Bauxilum the Caustic Molar Ratio (CMR) is defined as: CMR = 1.645 * [Na2O]/[Al2O3] where the constant 1,645 is: Al2O3 Molecular Weight/Na2O Molecular Weight and the changes of this expression are produced specially in the agglomeration stage. The following work shows the difference in the behavior among agglomeration and growth stages and influence of the total caustic and the impurities levels on the changes of CMR, especially during the agglomeration stage of the precipitation circuit. The effect of the major impurities and its relations to the total caustic and occluded soda were analyzed through empirical equations by means of statistical programs. The effects of variables that influence the precipitation circuit productivity were also determined.

9:20 AM
Effect of Residual Hydrate on Properties of Metallurgical Grade Aluminas: *Miguel Ángel Llavona*[1]; *Roberto Zapico Amez*[1]; [1]University of Oviedo, Dept. Matls. Sci., Gonzalo Gutiérrez Quirós s/n, Mieres, Asturias 33600 Spain

There are different types of water in metallurgical grade aluminas: physically adsorbed, chemisorbed, water of constitution and lattice water, and the aluminium industry uses several tests to determine it. If the moisture of the aluminas is determined to 110°C-4h, the MOI to 300°C-4h and the LOI to 1200° C-2h, according to the standard tests, and the alumina contains hydrate, the values of the MOI and LOI will be seen altered, and they will not have meaning. The loss of weight to 500°C has been related with the content in hydrate in the metallurgical grade aluminas. Thermal conductivity of aluminas have been determined by the hot wire method. A linear relation between thermal conductivity and density was observed. If the alumina has some residual hydrate, the obtained value of the thermal conductivity will be lower than the expected according with the packing density.

9:45 AM
Study on the Relationship Between the Stress-State and the Intensity of the Overlapped Al(OH)3 Crystals: Wangxing Li[1]; Lusheng Ye[2]; Shugui Hua[1]; Zhoulan Yin[1]; [1]Zhengzhou Research Institute of Chalco, Zhengzhou, Henan 450041 China; [2]Central South University, Physl.-Chmst. Inst., Changsha, Hunan 410083 China

Using stress analysis, the stress-state between two overlapped Al(OH)3 crystals was calculated. The relationship between the intensity and the overlap of the crystals was obtained. Conclusions were made that the intensity of two overlapped Al(OH)3 crystals is reduced as the overlap area is decreased. The method can also be used to study the relationship between the stress-state and the intensity for more overlapped Al(OH)3 crystals.

10:10 AM Break

10:25 AM
Influence of Organic Additives on Particle Size and Strength of Hydrate from Carbonization of Seeded Sodium Aluminate Liquors: *Wang Zhi*[1]; Bi Shiwen[2]; Yang Yihong[2]; Yuan Zhangfu[1]; [1]Chinese Academy of Sciences, Inst. of Process Engrg., Zhong Guan Cun, Haidian Dist., Beijing 100080 China; [2]Northeastern University, Sch. of Matls. & Metall., Wenhua Rd., Heping Dist., Shenyang, Liaoning 110004 China

Poor strength and excessive fine grain content are the main problem to be solved in the Sintering process for sandy alumina production. A systematic study was made of the effects and mechanism of different organic compounds on product median diameter and attrition index quantitatively and on the crystal habit of gibbsite qualitatively. It has been determined that some additive at certain concentration can significantly decrease the fine particle content, improve the product strength and modify gibbsite crystal morphology as crystal habit modifier. For instance, additive CF2 increases $Al(OH)_3$ median size by 12 μm at 200 ml/l, at the same time decreases the <45 μm particle mass fraction and the attrition index by 17% and 10% respectively. The enhancement of anti-attrition ability can be linked to the changes of structure and shape of gibbsite crystals. The crystal morphologies indicate that additives can accelerate the aggregation and inter-growth of crystal units, as a result the gibbsite presents an inlaid crystal structure close to globular shape.

10:50 AM
Application of Fractal Theory in Studying Strength of Sandy Alumina: *Tan Jun*[1]; Chen Qi Yuan[1]; *Yin Zhou lan*[1]; [1]Central South University, Chmst. & Cheml. Engrg., Lushan nanlu 154#, Changsha, Hunan 410083 China

The fractal theory was introduced to study the relationship of sandy alumina between morphology and strength. Morphological characterizations of a series of alumina from seeded and carbonization precipitation were described using scanning electron microscopy (SEM). Attrition indices and fractal dimensions were determined. It showed that the attrition index of alumina from carbonization precipitation increases with increasing fractal dimension. As to alumina from seeded precipitation, it suggested that the crystal structure should be considered during analyzing the relationship between fractal dimension and strength. The attrition index of alumina with the same structure increases with increasing fractal dimension.

11:15 AM
Microstructure Analysis of Aluminum Hydroxide and Alumina: Tan Jun[1]; *Chen Qi Yuan*[1]; *YIn Zhou lan*[1]; [1]Central South University, Coll. of Chmst. & Cheml. Engrg., Lushan nanlu 154#, Changsha, Hunan 410083 China

The microstructure of aluminum hydroxide and alumina were characterized by scanning electronic microscopy (SEM). The differences between two kinds of alumina from seeded precipitation and carbonization precipitation were compared. Two methods of breakage were developed to view the interior microstructure of alumina. The microstructure of alumina is similar to that of aluminum hydroxide, while there are some cracks on the surface of alumina. The small crystals to form alumina from seeded and carbonization precipitation are hexagonal prism, short hexagonal cylindrical respectively. The growth mechanism of aluminum hydroxide can be concluded according to the interior structure of alumina.

Aluminum Reduction Technology: Fundamentals

Sponsored by: Light Metals Division, LMD-Aluminum Committee
Program Organizers: Tor Bjarne Pedersen, Elkem Aluminium ANS, Farsund 4551 Norway; Tom Alcorn, Noranda Aluminum Inc., New Madrid, MO 63869 USA; Halvor Kvande, Norsk Hydro ASA, Oslo N-0240 Norway

Thursday AM Room: 2003
February 17, 2005 Location: Moscone West Convention Center

Session Chair: Pavel Fellner, Slovak University of Technology, Inorganic Tech., Bratislava SK-812 37 Slovakia

8:30 AM
A New Modelling for Simulating Bubble Motions in a Smelter: *Michel V. Romerio*[1]; Alexei Lozinski[1]; Jacques Rappaz[1]; [1]Swiss Federal Institute of Technology, IACS, Lausanne 1015 Switzerland

A model allowing to describe motion, coalescence and escape of bubbles in the bath under the action of gravitation is proposed. The bubbles introduced under the anodes at the initial time have fixed sizes corresponding to those obtained by the detachment phenomenon. Bubble shapes are described by ellipsoids with a fixed volume. The gas motion effects inside the bubbles are neglected. The motion of a bubble is obtained in a Lagrangian form using the virtual works principle. It is thus described by the motion of the gravity center combined with a rotation and a deformation. The set of equations is numerically solved with the help of the fictitious domain technique in which the Navier-Stokes equations in the domain formed by both fluid and gas are considered. The equations governing the bubbles motion are imposed by introducing Lagrange multipliers on the bubbles boundaries. Numerical results in 2D are presented.

8:55 AM
Experimental and Numerical Studies on Bubble Removal Under Anodes by Using Ultrasound in Water Solutions and in Cryolitic Melts: Harald A. Øye[1]; *Jilai Xue*[1]; G. Servant[1]; Trygve Foosnæs[1]; [1]Norwegian University of Science and Technology, Dept. of Matls. Tech., Sem Sælands v. 14, Trondheim N-7491 Norway

Gas bubbles under the anodes during aluminium electrolysis constitute a significant part of the cell voltage drop, and large bubbles can sometimes result in unwanted anode effects. Laboratory studies on removing gas bubbles under anodes by using ultrasound were carried out in water solutions and in cryolitic melts. Numerical simulation techniques were applied in scale- up of the anode size. With 20 kHz and 28 kHz ultrasound, the gas bubbles are removed from the downward surface of the anodes, which result in a reduction in the cell voltage. The results show potential in energy saving, while the ultrasound effectiveness should be improved before possible application of this technology in aluminium reduction cells.

9:20 AM
Simulation of the Bubble Layer in Aluminum Electrolysis Cells: *Laszlo I. Kiss*[1]; Sándor Poncsák[1]; Jacques Antille[2]; [1]Universite du Quebec, Dept. des Scies. Appliquees, 555, boul. de l'Universite, Chicoutimi,

Quebec G7H 2B1 Canada; [2]Alcan Primary Metals Europe, Sierre CH 3695 Switzerland

The structure and dynamics of the bubble laden layer has an important influence on the performance of the aluminum reduction cells as the gas bubbles block the way of passage of the electric current. The extent of the gas covered portion of the anode bottom depends on the equilibrium between the rates of production and evacuation of the gas. A mathematical model was developed that predict the variation of the covering factor as a function of the design and operational parameters of the aluminum electrolysis cell. The simulator offers the time series of the fluctuations of the covering factor, its average values as well as a graphical representation of the movement of the bubbles. The influence of the size and shape of the anode on the covering factor is presented.

9:45 AM
Regimes of the Movement of Bubbles Under the Anode in an Aluminum Electrolysis Cell: *Alexandre Perron*[1]; László I. Kiss[1]; Sándor Poncsák[1]; [1]Université du Québec à Chicoutimi, Dept. des Scis. Appliquees, 555 boul. de l'Université, Chicoutimi, Québec G7H 2B1 Canada

Although the bubble layer plays and important role in the operation of an aluminum reduction cell, the details of the nucleation, detachment and movement of the bubbles are not completely understood. The direct observation of the bubble related phenomena is practically impossible, so our understanding is based on theoretical analysis, speculative models and on the observation of the behavior of bubbles in water models or in other low temperature, transparent systems. In the present paper the different regimes of the movement of the individual bubbles under a downward facing solid plate are discussed. The formation of a separating liquid layer, the kinematics of the bubbles as well as the flow field around them were observed and analyzed using low temperature physical models.

10:10 AM
A New Study on Bubble Behaviors on Carbon Anode in Aluminum Electrolysis: *Bingliang Gao*[1]; Zhaowen Wang[1]; Zhuxian Qiu[1]; Haitao Li[1]; [1]Northeastern University, Coll. of Matls. & Metall., MB 117, Shenyang, Liaoning 110004 China

In this paper, the bubble behaviors on carbon anodes during aluminum electrolysis were studied in a bench scale cell. Previous studies on anode bubble behaviors were largely based on the water models simulation and see-through electrolysis cell observation. The tests adopted same method used by R.J Aaberg to investigate the influence of anode current density and anode-cathode distance (ACD) on the anode bubble behaviors at the status of electrolysis. PLC (programmable controller) combined with a computer was applied to collect experimental data. The results of the study indicate: Increasing current density leads to increasing release frequency of bubbles and thin bubble layer thickness when current density on anode is less than 1.2A/cm2; At higher anode current density, the release frequency of the anode bubbles decreases with increasing current density; During anode effect, the release frequency of the anode bubbles goes to zero.

10:35 AM Break

10:50 AM
Chemical and Electrochemical Reactions of Sulphur Species in Cryolite Melts: *Pavel Fellner*[1]; Marta Ambrová[1]; Ján Híves[1]; Michal Korenko[2]; Jomar Thonstad[3]; [1]Slovak University of Technology in Bratislava, Dept. of Inorganic Tech., Radlinskeho 9, Bratislava SK - 812 37 Slovakia; [2]Slovak Academy of Sciences, Inst. of Inorganic Chmst., Dúbravská cesta 9, Bratislava SK-845 38 Slovakia; [3]Norwegian University of Science and Technology, Dept. of Matls. Tech., Trondheim N-7491 Norway

Data on the chemical reduction of sulphate by aluminium and by graphite in cryolite melts will be reported. Chemical reduction of sulphate by aluminium or carbon follows a similar sequence. Only SO42-, S2- and polysulphides species were detected in the solidified melts. It was found that sulphide reacts with dissolved iron(II), forming FeS, which is insoluble in cryolite melts. Because of its high density, solid FeS particles will tend to settle and react with the aluminium cathode, forming Al2S3, which is readily soluble in molten cryolite. This may be a non-electrochemical mechanism for contaminating aluminium with iron. The cryolite-rich part of the phase diagram Na3AlF6-Al2S3 was determined. By cathodic reduction of sulphate it was found that two electrons take part in the reduction of sulphate, i.e. SO42- + 2e- = SO32- + O2-. Since the sulphite species is not stable at high temperatures, it decomposes thermally into SO42-and S2-.

11:15 AM
Aluminum Electrowinning in Ionic Liquids at Room Temperature: *Mingming Zhang*[1]; Venkat Kamavaram[1]; Ramana G. Reddy[1]; [1]University of Alabama, Metallurgl. & Matls. Engrg., A-129 Bevill Bldg., 126 Seventh Ave., PO Box 870202, Tuscaloosa, AL 35487-0202 USA

The electrowinning of aluminum was studied in room temperature ionic liquids prepared by mixing 1-hexyl-3-methylimidazolium chloride (C6mim[Cl]) and aluminum chloride (AlCl3). Aluminum was electrowinned at copper cathode with graphite as anode. Cathode current density and current efficiency increase with increasing temperature, molar ratio of AlCl3 and applied cell voltage. However, high current efficiencies were obtained at high voltage, intermediate AlCl3 concentration and low temperature. The deposit morphology and thickness were examined in detail using SEM and XRD techniques. The electrowinning of aluminum in C6mim[Cl]-AlCl3) and C4mim[Cl]-AlCl3 was also compared regarding the current density and current efficiency.

11:40 AM
The Aluminum Reduction Cell Closed System of 3D Mathematical Models: Gennady V. Arkhipov[1]; *Alexander V. Rozin*[2]; Alexander G. Arkhipov[1]; [1]RUSAL, Engrg.-Technologl. Ctr. Ltd., Pogranichnikov St. 37, Krasnoyarsk 660111 Russia; [2]Lomonosov Moscow State University, Inst. of Mech., Michurinsky Pr. 1, Moscow 119899 Russia

3D mathematical models to predict different processes in aluminum reduction cell have been developed by RUSAL for several recent years. Each of the models can calculate the field of some physical parameter (e.g. flow velocity) using for data fields of other parameters (current density and magnetic induction) or boundary conditions (ledge profile) produced by other models. In this study all models have been worked out to run simultaneously except for the calculation of magnetic field, which is assumed to be stationary. Natural convection and radiation are taken into account in the conjugate heat transfer problem. This closed system of mathematical models makes possible to evaluate main physical parameters in the reduction cell but it needs large computation times. To solve the optimization tasks simplified "local" models can be created based on the coarse-mesh solutions of the whole problem.

Bulk Metallic Glasses: Mechanical Behavior and Phase Transformation

Sponsored by: Structural Materials Division, SMD-Mechanical Behavior of Materials-(Jt. ASM-MSCTS)
Program Organizers: Peter K. Liaw, University of Tennessee, Materials Science and Engineering, Knoxville, TN 37996-2200 USA; Raymond A. Buchanan, University of Tennessee, Materials Science and Engineering, Knoxville, TN 37996-2200 USA

Thursday AM Room: 3006
February 17, 2005 Location: Moscone West Convention Center

Session Chairs: Yoshihiko Yokoyama, University of Hyogo, Matls. Sci. & Engrg., Himeji 671-2201 Japan; D. H. Kim, Yonsei University, Metallurgl. Engrg., Seoul 120-749 S. Korea

8:30 AM
Development and Characterization of New Ca-Mg-Zn-Cu Bulk Metallic Glasses: *Oleg N. Senkov*[1]; J. Mike Scott[1]; [1]UES, Inc., Matls. & Processes Div., 4401 Dayton-Xenia Rd., Dayton, OH 45432 USA

Several Ca-Mg-Zn-Cu bulk metallic glasses with the thickness of up to 10 mm were produced by a Cu mold casting method. The glass transition, crystallization, solidus and liquidus temperatures, as well as the heats of crystallization and melting were determined for these glasses using differential scanning calorimetry. Compression properties of these amorphous alloys were also studied at room temperature and in the temperature range of the super-cooled liquid (ΔT_x range). As-cast alloys were very brittle at room temperature; however, ~30-40% compression strain was recorded during elevated temperature deformation. After deformation in the ΔT_x range the alloys remained fully amorphous and they showed some ductility at room temperature.

8:50 AM
Modeling the Formability of Bulk Metallic Glasses: *Justin Cheney*[1]; Kenneth S. Vecchio[1]; [1]University of California, Dept. of MAE, Matls. Sci. Grp., 9500 Gilman Dr., La Jolla, CA 92093-0411 USA

Understanding the processes of glass formation in metals will allow better alloys with lower critical cooling rates to be produced. Lowering the critical cooling rate includes slowing the crystallization rates of metal alloys through kinetic and thermodynamic means. Currently no definitive method for evaluating the theoretical glass forming ability of an alloy has been produced. In the current work, liquidus surfaces are generated using ThermCalc simulations to determine deep eutectics in multi-component alloys. Three-dimensional visualization is used to examine the melting temperatures of an entire compositional range within a multi-component alloy. The thermodynamic behavior of an alloy is evaluated with this technique as the crystal nucleation temperature follows the trend of the liquidus temperature. To model the kinetics of amorphous forming ability, a short range order simulation in combination with random hard sphere packing models are used. The result gives a theoretical description of the atomic movement necessary to form a crystal structure. The aim is to predict alloys that can exist as densely packed liquids with uniformly distributed, large magnitude strain fields. 3-D visualization of the model predictions is used to evaluate the theoretical structures of an alloy, in addition to the strain fields and packing densities that exist throughout the volume. These models are compared with existing empirical data to confirm their validity. The simulations can then be used to evaluate all possible elemental combinations to determine potentially novel alloy systems with higher glass forming ability.

9:10 AM
Mg49Y15Cu36 Bulk Metallic Glass Composites Synthesized by Vacuum Hot-Pressing of Mechanically Alloyed Powders: *Pee-Yew Lee*[1]; Cheng Lo[1]; [1]National Taiwan Ocean University, Matls. Engrg., 2, Pei-Ning Rd., Keelung, Taiwan 202 Taiwan

In the present study, WC/Mg49Y15Cu36 metallic glass composite powders were prepared by mechanical alloying of pure Mg, Y, Cu, and WC powder mixtures. Mg49Y15Cu36 metallic glass composite powders were obtained after 10 h of milling as confirmed by X-ray diffraction and differential scanning calorimetry. The metallic glass composites powders were found to exhibit a supercooled liquid region before crystallization. Bulk metallic glass (BMG) composites were synthesized by vacuum hot pressing the as-milled Mg49Y15Cu36 metallic glass composite powders at 723 K in the pressure range of 0.72-1.20 GPa. BMG composite with submicron WC particles homogeneously embedded in a highly dense nanocrystalline/amorphous matrix was successfully prepared under applied pressure of 1.20 GPa. It was found that the pressure could enhance the thermal stability and promotes nanocrystallization of WC/Mg49Y15Cu36 BMG composites.

9:30 AM
Transformations Near the Glass Transition in Pd-Based Bulk Metallic Glasses: *Shantanu Vijay Madge*[1]; Gerhard Wilde[1]; [1]Forschungszentrum Karlsruhe, Inst. of Nanotech., Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen 76344 Germany

Bulk metallic glasses (BMGs) are interesting partly because of the complexity that underlies crystallisation in these alloys, which can involve various metastable intermediate phases. Phase separation in the undercooled liquid is an issue that has seen much attention in recent years in order to explain the counter-intuitive nanocrystallisation that occurs in some BMGs. In the present work, a series of Pd-based BMGs has been prepared by suction-casting. The transformations in certain glasses on heating above the glass-transition temperature are investigated by complementary techniques such as modulated-temperature calorimetry, X-ray scattering and transmission electron microscopy. The results are discussed in the light of possible amorphous phase separation that has been suggested to occur also in Pd-rich systems. The possibility of using phase separation for preparing glass-glass composites with enhanced mechanical properties is also considered.

9:50 AM
A New Criterion for Glass Forming Ability of Bulk Metallic Glasses: *E. S. Park*[1]; W. T. Kim[2]; D. H. Kim[1]; [1]Yonsei University, Dept. of Metallurgl. Engrg., Ctr. for Non-Crystalline Matls., 134 Shinchon-Dong, Seodaemun-gu, Seoul 120-749 S. Korea; [2]Chongju University, Dept. of Applied Sci., 36, Naedok-Dong, Sangdang-Gu, Chongju, Chungbuk 360-764 S. Korea

A new criterion for glass forming ability (GFA) of bulk metallic glasses (BMGs) is proposed based on the consideration of both the liquid phase stability and the resistance to the formation of competing crystalline phases. Especially, the simple rule of mixtures of melting temperatures,Tmmix has been considered for a comprehensive expression to predict GFA for various glass-forming systems. The interrelationship between this new parameter and maximum diameter, Dmax is elaborated and discussed in comparison with four other representatives, i.e. supercooled liquid region, K parameter, reduced glass transition temperature Trg, and gamma parameter. The new parameter demonstrates the highest regression coefficient value and the narrowest prediction band implying that the new parameter correlates better with the maximum diameter, Dmax than other parameters suggested so far. It is therefore considered that the presently proposed parameter has a stronger correlation with GFA in the various BMG alloy systems.

10:10 AM
Evaluation of Shear Bands Developed Under the Tensile Deformation Mode for Bulk Metallic Glasses and MMCs Reinforced by Metallic Glass: *Donghyun Bae*[1]; [1]Yonsei University, Dept. of Metallurgl. Engrg., 134 Shinchon-dong, Seodaemun-gu, Seoul 120-749 Korea

The tensile deformation/failure behaviors of a Zr-based bulk metallic glass (BMG) and metal matrix composites (MMCs) reinforced by Ni-based metallic glass fibers have been systematically investigated. The Zr-based BMG is fabricated by the suction casting method and the MMCs are synthesized by warm extrusion of gas-atomized powders. Under the tensile loading conditions, i.e. 4-point bending or uniaxial tension, the shear bands are developed significantly due to the constrained effect stemming from strain distribution for 4-point bending or from confinement of ductile matrix for MMCs. The formation and propagation of the shear bends under tension, significantly different from those observed under compression, and its structure will be discussed.

Carbon Technology: Cathode Materials and Corrosion II

Sponsored by: Light Metals Division, LMD-Aluminum Committee
Program Organizers: Todd W. Dixon, ConocoPhillips, Borger, TX 79007 USA; Halvor Kvande, Norsk Hydro ASA, Oslo N-0240 Norway; Markus Meier, R&D Carbon, Sierre CH 3960 Switzerland

Thursday AM Room: 2007
February 17, 2005 Location: Moscone West Convention Center

Session Chair: Morton Sorlie, Elkem Aluminium ANS Research, Dept. of Matls. Tech., N-4675 Kritiansand Norway

8:30 AM
Quality Evaluation of Nitride Bonded Silicon Carbide Sidelining Materials: *Egil Skybakmoen*[1]; Lisbet Stoen[1]; Jannicke H. Kvello[1]; Ove Darell[1]; [1]SINTEF Materials and Chemistry, Energy Conversion & Matls., Sem Saelandsvei 6, Trondheim N-7465 Norway

A laboratory test method to determine the chemical/oxidation resistance of commercially available SiC-based sidelining materials was developed at SINTEF in 1996. Since then more than 260 samples from around 20 suppliers world-wide have been tested, and an overview of typical - and abnormal results will be given. The tests have demonstrated the importance of checking the quality of the SiC blocks throughout the entire cross section of the blocks. Large variations were found, depending on whether samples were taken near the surface or from the central parts of the blocks. The observed degradation will be discussed in terms of a proposed reaction mechanism, and related to material quality parameters and test conditions (bath acidity and gas atmosphere).

8:55 AM
Effect of Changes in Physical-Mechanical Properties of Materials on Aluminum Reduction Cell Performance: *Gennady V. Arkhipov*[1]; Victor Yu. Buzunov[1]; Vitaly V. Pingin[1]; Vasily I. Borisov[1]; [1]RUSAL, Engrg.-Technologl. Ctr. Ltd., Pogranichnikov St. 37, Krasnoyarsk 660111 Russia

Calculation results of thermo-electric-mechanical fields with the initial lining and cathode shell material properties differ numerically from calculated results taking into account the property changes during operation. Mathematical modeling demonstrated effects of changes in the properties on thermoelectric fields, magnetic hydrodynamics and stress-strain state. To study changes in properties like electric conductivity, thermal conductivity, elasticity modulus, thermal and sodium expansion of lining materials, they have been investigated after autopsies of cells with different life. Mechanical properties of cathode shells have been investigated after different campaigns to study changes in mechanical properties of the steel.

9:20 AM
Titanium Diboride and Molybdenum Silicide Composite Coating on Cathode Carbon Blocks in Aluminum Electrolysis Cells by Atmospheric Plasma Spraying: *Huimin Lu*[1]; Ruixin Ma[1]; Wenhui Yuan[1]; Yongheng Wang[1]; [1]University of Science and Technology, Metallurg. Engrg. Sch., No. 30 Xueyuan Rd., Beijing, Beijing 100083 China

Self-propagating high-temperature synthesis with reduction process was used to fabricate the TiB2- MoS2 composite powder. The TiB2- MoS2 composite was coated on the cathode carbon blocks by atmospheric plasma spraying. Various properties of the coated carbon block such as the chemical and electrochemical stability, the corrosive resistance, thermal shock resistance, wettability and service life in molten cryolite-alumina and aluminum liquids were tested. The microstructure of the coating, the interfacial bonding between the coating and the carbon substrate, thermal expansion performance and electrical resistivity of the coating, the effect of different process parameters e.g. spray distance, additive MoS2 content on the coating were also studied. These research results indicate that the TiB2-MoS2 composite coating cathodes by atmospheric plasma spraying have the potential to give significant benefits to the aluminum electrolysis process in terms of energy coast saving and extended cell life.

9:45 AM
The Effect of Sodium-Containing Additives on the Sodium-Penetration Resistance of TiB2/C Composite Wettable Cathode in Aluminum Electrolysis: *Qingyu Li*[1]; Yanqing Lai[2]; Jie Li[2]; Jing Fang[2]; Jianhong Yang[2]; Zhu Chen[3]; [1]Guangxi Normal University, Sch. of Chmst. & Cheml. Engrg., Guilin, Guangxi 541004 China; [2]Central South University, Sch. of Metallurgl. Sci. & Engrg., Changsha, Hunan 410083 China; [3]Aluminum Corporation of China Limited, Guangxi Branch, Pingguo, Guangxi 431400 China

TiB2/C composite material is one of the best wettable cathode materials for aluminum electrolysis. But TiB2/C composites usually contain about 30-70% carbon, which results in the expansion and failure of the composites due to sodium and bath penetration in aluminum electrolysis. In this paper, TiB2/C composites were prepared with sodium-containing additives, such as spent potlining powder, as carbon component hoping to improve the sodium-penetration resistance of TiB2/C composites in aluminum electrolysis. Results showed that the sodium-penetration resistance of TiB2/C composites in aluminum electrolysis was improved effectively by adding sodium-containing additives.

10:10 AM Break

10:25 AM
Cells Incorporating Cathode Blocks Impregnated with Boron Oxide: *Rudolf Keller*[1]; [1]EMEC Consultants, 4221 Roundtop Rd., Export, PA 15632 USA

Cathode blocks of aluminum reduction cells were impregnated with boron oxide. The purpose was to promote the wetting of the carbon surface by aluminum metal with the formation of titanium diboride through the reaction of the boron oxide with titanium being added to the metal pool. An 11-month test with a cell fully equipped with impregnated amorphous blocks (containing 30% graphite) resulted in excellent, minimal cathode wear, but it did not yield operational benefits. It is projected that the approach is very promising for use with graphitized blocks, particularly to improve cathode life. This presentation is based on work conducted in cooperation with industrial partners (Century Aluminum, Northwest Aluminum, and SGL Carbon) and supported by the Department of Energy under Cooperative Agreement DE-FC36-98ID13664.

10:50 AM
Effect of Porosity Structure on Penetration and Performance of Lining Materials: *Sergey A. Khramenko*[1]; Peter V. Polyakov[2]; Alexander V. Rozin[3]; Alexander P. Skibin[4]; [1]RUSAL Engineering & Technology Centre, Pogranichnikov St. 37, Krasnoyarsk 660111 Russia; [2]State University for Non-Ferrous Metals and Gold, Krasnoyarskiy Rabochiy St.95 66025 Russia; [3]Lomonosov Moscow State University, Inst. of Mech., Michurinsky Pr. 1, Moscow 119899 Russia; [4]Bauman Moscow State Technical University, Profsouznaya St.100-4-40, Moscow 117437 Russia

The characteristic property of cathode materials is porosity that causes bath penetration in the cathode blocks. As a result, internal stresses and micro cracks may appear that increase the wear of the reduction cell. The pore distribution in the cathode blocks materials from different manufactures is investigated. It is found that pore distributions vary from homogeneous monopore normal distribution of pore size to bipore distribution and even nonuniform structure with continuous distribution of pores. The mechanism of pores formation is investigated experimentally on the model patterns of cathode carbon materials. The dependences of their physical and engineering attributes on pore structure are obtained. The mathematical model of the bath filtration in the cathode blocks during start up operations is created. The model can estimate the performance attributes of the cathode materials with different pore structure and its influence on cell lifetime.

Cast Shop Technology: Foundry

Sponsored by: Light Metals Division, LMD-Aluminum Committee
Program Organizers: Gerd Ulrich Gruen, Hydro Aluminium AS, Bonn 53117 Germany; Corleen Chesonis, Alcoa Inc., Alcoa Technical Center, Alcoa Center, PA 15069 USA; Halvor Kvande, Norsk Hydro ASA, Oslo N-0240 Norway

Thursday AM — Room: 2001
February 17, 2005 — Location: Moscone West Convention Center

Session Chair: Arne K. Dahle, University of Queensland, CRC for Cast Metals Mfg., Brisbane Qld 4072 Australia

8:30 AM
Simulation of Microstructures and Yield Strength of a High Pressure Die Cast A380 Aluminum Alloy Component: *Mei Li*[1]; Jake Zindel[1]; Larry Godlewski[1]; Brian Schneider[1]; Adam Olukalns[1]; Christopher M. Wolverton[1]; John Allison[1]; [1]Ford Motor Company, Ford Rsch. & Advd. Engrg. Lab., 2101 Village Rd., Dearborn, MI 48124 USA

Cast aluminum alloys are increasingly being utilized by automotive industry for manufacturing chassis and powertrain components to reduce vehicle weight and consequently increase fuel economy and reduce emissions. High pressure die casting process provides tremendous cost saving opportunities in manufacturing these components. Development of Virtual Casting tools for HPDC aluminum will lead to fast prototyping and tooling, thus fast final products with reduced cost. This talk describes the development of the interfacial heat transfer coefficients between casting and die with in-cavity and in-die thermal couple measurements in a lab HPDC component, the simulation of microstructure evolution during casting and the prediction of yield strength of an engine block. The prediction can be used to design and optimize casting component and process.

8:50 AM
Preliminary Results on the Effects of Modification During Semi-Solid Processing of Al-Si Alloys: *Shahrooz Nafisi*[1]; [1]University of Quebec, CURAL, 555, Univ. Blvd., Chicoutimi, Quebec G7H 2B1 Canada

Silicon is one of the most important alloying elements incorporated in aluminum alloys. Its addition is to improve castability, fluidity, reduce shrinkage as silicon expands on solidification and renders superior mechanical properties. The morphology of silicon however plays an important role on the properties of finished products. Therefore, the usual practice is to modify the as-cast flake or acicular silicon morphology employing special heat treatment or addition of certain modifiers. As a result, the silicon morphology changes to fibrous form and thus the mechanical properties of the as-cast parts improve. For conventional casting, this treatment has been investigated widely by so many researchers but in the SSM processing, few published papers could be found. In this article, the addition of Sr as a modifier for Al-Si binary alloy is investigated for semi-solid alloy using the patented SEED process, "Swirled Enthalpy Equilibration Device."

9:10 AM
Effects of Sr-Na Interactions in Hypoeutectic Foundry Alloys: *Liming Lu*[1]; Malcolm J. Couper[2]; Arne K. Dahle[1]; [1]University of Queensland, CRC for Cast Metals Mfg., Sch. of Engrg., Brisbane, QLD 4072 Australia; [2]Comalco Research & Technical Support, 15 Edgars Rd., Thomastown, VIC 3072 Australia

From recent published data, it is still unclear whether combined additions of Na and Sr have synergistic effects or deleterious interactions. This paper clarifies the interactions and the effects on alloy solidification and castability. Combined additions of Sr and Na do not appear to cause improvement of the modification of the eutectic microstructure even after only a short period after addition. Na addition may promote Sr vaporization and/or oxidation kinetically, leading to a quicker loss of both modifiers, which is blamed for the disappearance of the modification effect during holding. Quenching trails during the eutectic arrest indicate that addition of Sr into Na-modified melts does not alter the eutectic solidification behaviour. The effect of

Na on eutectic solidification dominates, and the eutectic is observed to evolve with a significant dependency on the thermal gradient. Combined Sr and Na additions produced no beneficial effects on porosity and casting defects.

9:30 AM
Dissolution, Recovery and Fade of Sr Master Alloys in Al-7Si-0.5Mg Casting Alloy: *John A. Taylor*[1]; Malcolm J. Couper[2]; Catherine L. Smith[2]; Darius P.K. Singh[3]; [1]University of Queensland, CRC for Cast Metals Mfg. (CAST), Sch. of Engrg., Brisbane, QLD 4072 Australia; [2]Comalco Research and Technical Support, 15 Edgars Rd., Thomastown, VIC 3074 Australia; [3]Ion Automotive, 100 Plunkett Ave., Manukau City, Auckland New Zealand

A number of commercial Al-Sr master alloys of differing Sr content and product form have been added to Al-7Si-0.5Mg casting alloy melts and held at constant temperature for periods of at least 6 hours following the addition. The master alloys were added to achieve specific Sr target levels (mostly 200 ppm, but also 500 and 1,000 ppm) and the melts were held at various temperatures (most at 710ºC, but also 670, 690, 740 and 770ºC). A total of thirty six melt trials were conducted and during each trial chill-cast disc samples were taken throughout for subsequent chemical analysis. The Sr concentration versus time data of each trial has been considered in terms of Sr dissolution/recovery behaviour, as well as Sr loss/fade. Trends in the data are identified and discussed, and implications for industrial practices are suggested.

9:50 AM
Effect of Process and Design Variables in the Production of Expandable Polystyrene Patterns for Lost Foam Casting: *Rohan Bhat*[1]; Sushil Bhavnani[1]; Ruel Overfelt[1]; David Sheldon[2]; [1]Auburn University, Mechl. Engrg., 201 Ross Hall, Auburn, AL 36832 USA; [2]Vulcan Engineering Company, Helena, AL 35080 USA

The defects caused in Lost Foam Casting (LFC) are believed to be due to inconsistencies in the Expandable Polystyrene (EPS) pattern injection process. It is believed that fairly small localized density variations in EPS patterns lead to folds and other casting defects. The focus of this study is to understand the cause of these inconsistencies. The packing of EPS beads into the mold during a pattern-making is affected by system parameters such as the fill pressure and the pressure in the bead supply canister, geometric features such as distance between the tip of injector and the surface on which beads impinge, and the venting configuration. High speed video confirms that the time required for the mold to get packed with beads affects the density distribution; especially when used with a pressurized bead canister. For injector to opposing wall (IOW) distance less than 3.5mm, the injector performance becomes erratic. It was observed that for IOW distance less than 8mm the density gradient within the mold was about 12% for a vented bead canister and was about 16% for pressurized canister operation. As the IOW distance increases the density distribution throughout the mold gets better. The bead mass dispensed increased with increase in both fill pressure and canister pressure leading to an increase in the packing ratio (defined as the ratio of volume occupied by beads to total mold volume). Pressure measurements at the injector tip and the vent locations are also reported. The fill time decreased as the pressure increased but was independent of fill pressure at high canister pressure. With this better understanding of the blowing process in LFC, mold designers can design molds which produce better patterns leading to the production of sound quality castings.

10:10 AM Break

10:20 AM
Effect of Flux Compositions on Grain Refinement in Al-Si-Mg Alloy: *Chaowalit Limmaneevichitr*[1]; Witthaya Eidhed[2]; [1]King Mongkut's University of Technology Thonburi, Production Engrg. Dept., 91 Pracha-u-tit Rd., Bangmod, Tungkhru, Bangkok 10140 Thailand; [2]King Mongkut's Institute of Technology North Bangkok, Faculty of Engrg., Bangsue, Bangkok 10800 Thailand

There are many compositions in fluxes and each composition has different effects on melt treatment. However, the effect of flux compositions on grain refinement fading has not yet been well established. This research is to study effect of different typical chemical compositions in various ratios on grain refinement fading after recycling of return scraps. Al-Si-Mg alloy (A356) was selected for this research and grain refined using 0.2 wt. % of Al-5Ti-1B grain refiners. Each molten alloy was treated with three different fluxes at 1% of aluminum weight. The work was undertaken by recycling the grain-refined castings for four cycles. No grain refiner was added but the same flux was added in each melting process at the same weight ratio. It was found that flux compositions have strong effect on grain size and fading phenomenon of grain refinement. Based on this result, it was found that MgCl2 in flux composition can reduce the fading phenomenon substantially.

10:40 AM
Effect of Stirring on the Morphological Evolution of Silicon in Al-Si Alloys: *Shahrooz Nafisi*[1]; [1]University of Quebec, 555, Univ. Blvd., Chicoutimi, Quebec G7H 2B1 Canada

SemiSolid Metal Processing (SSM) is a relatively new technology for metal forming different from the conventional forming process which use either solid or liquid metals as started materials. In SSM processing of AlSi alloys, there are two important features that should be considered, the size and shape of the primary á-Al particles and also the morphology of silicon in the eutectic phase. It is quite well known that the irregular growth of the Si eutectic can be modified by addition of modifiers, i.e., Strontium. In this paper, it will be shown that in the SSM processing with stirring application, not only á-Al particles took the rosette or globule shape, but also the silicon in the eutectic is broken and become much smaller in size.

11:00 AM
Impact of Cu Additions on a Structure and Mechanical Properties of Near and Hypoeutectic Silumins: *Tomasz Stuczynski*[1]; Zbigniew Zamkotowicz[1]; Marzena Lech Grega[1]; [1]Institute of Non-Ferrous Metals, Light Metals Dept., Pilsudskiego 19, Skawina 32-050 Poland

Paper presents results of investigations defining the role of Cu in forming macro and microstructure of near and hypoeutectic silumins. The following parameters acted as criteria of evaluation: size of grain and dendrites of solid solution á as well as the mechanical properties of tested alloys. Achieved results were presented to forecast the properties of alloys in a function of chemical composition.

11:20 AM
Study on Method of Increasing Viscosity in Fabricating Aluminum Foam: Hong-jie Luo[1]; G.C Yao[1]; [1]Northeastern University, Sch. of Matls. & Metall., Wenhua Rd., No.11, Heping Dist., Shenyang, Liaoning Province 110004 China

The method of directly foaming in molten Al to prepare closed-cell aluminum foam is described in this article. Different kinds of ingredients are put into the molten Al alloy to make its viscosity increased. The TiH2 as foaming agent is also added into these molten Al to fabricate aluminum foam. The effectiveness of the method to increase the viscosity of molten Al on foam structure is researched by macroscopic observation and microstructure analysis. The results are showed as follow. After these ingredients, such as calcium, magnesium, Al2O3 and coal ash, etc, had been added into molten Al, the phase component of Al alloy changed. However the phase component and the mechanism of its increasing viscosity is different slightly. Meanwhile, the obtained Al foam also has great difference in its structure. The foams obtained by calcium and coal ash hold thick cell wall and high intensity, while the foams obtained by magnesium and Al2O3 hold thin cell wall and low intensity.

Computational Thermodynamics and Phase Transformations: Phase Field Models and Related Methods

Sponsored by: Electronic, Magnetic & Photonic Materials Division, Materials Processing & Manufacturing Division, Structural Materials Division, EMPMD/SMD-Chemistry & Physics of Materials Committee, MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS)
Program Organizers: Corbett C. Battaile, Sandia National Laboratories, Materials and Process Modeling Department, Albuquerque, NM 87185-1411 USA; Christopher Mark Wolverton, Ford Motor Company, Scientific Research Laboratory, Dearborn, MI 48121-2053 USA

Thursday AM Room: 3005
February 17, 2005 Location: Moscone West Convention Center

Session Chair: Christopher Mark Wolverton, Ford Motor Company, Scientific Rsch. Lab., Dearborn, MI 48121-2053 USA

8:30 AM Invited
Bridging the Scales Between Thermodynamic, Microscopic and Macroscopic Calculations When Simulating Solidification Microstructures: *Peter D. Lee*[1]; Robert C. Atwood[1]; [1]Imperial College London, Matls., Prince Consort Rd., London SW7 2BP UK

Models of phase transformations have proved very beneficial when investigating microstructural features when the representative volume element (RVE) is only one or two orders of magnitude larger then the

spatial discretization required to encapsulate the relevant physics. However, during solidification in particular, microstructural features are formed through phenomena occurring over multiple length scales due to the interaction of crystallographic, thermodynamic, and diffusion processes. This limits the applicability of RVE techniques. Therefore other approximations must be made to bridge the scales and allow the influence of microstructural features on the final performance of engineering components to be simulated. This paper presents an approach to bridging these scales by combining thermodynamic data into a microscale model and then weakly coupling these results into macroscopic heat transfer models.

9:00 AM
Phase-Field Modeling of the Irregular Interface Morphology During Directional Solidification: *Taiming Guo*[1]; Guoxiang Wang[1]; [1]University of Akron, Dept. of Mechl. Engrg., Akron, OH 44325-3903 USA

Depending on the relative strength of the anisotropy of the surface tension, a growing solidification interface may develop into various distinguished patterns. This paper employs the phase-field model with both the anisotropy of the surface tension and the anisotropy of the kinetic attachment to simulate such interface patterns observed in the directional solidification experiments. Not only the regular interface patterns (planar, cellular and dendritic patterns), but also the irregular interface patterns (tilted dendritic, degenerate, seaweed, doublon and doublet) have been successfully reproduced. The parameters of the temperature gradient, the anisotropy of the surface tension, the anisotropy of the kinetic attachment and the tilt angle are studied in the model. It has been found that the irregular interface patterns occur with a weak anisotropy of the surface tension and is strongly affected by the anisotropy of the kinetic attachment. On the basis of the simulation results, a morphology diagram is constructed with respect to the anisotropy of the surface tension and the anisotropy of the kinetic attachment.

9:20 AM
Online-Coupling of Thermodynamic Databases to a Multi-Phase-Field Model - Application to Hypereutectic Aluminum Casting Alloys: *Bernd Böttger*[1]; Ingo Steinbach[1]; [1]ACCESS e.V., Intzestr. 5, Aachen 52072 Germany

Due to the increasing computer performance phase-field methods allow more and more realistic microstructure simulations for practical foundry problems. If many alloy components and different phases are involved the exact description of the thermodynamic properties becomes absolutely critical for getting realistic simulation results. Ideal solution approximations, linear phase diagrams or tie-line tables are helpful only in special cases. In this conference paper the online-coupling of CALPHAD-databases to the phase-field software MICRESS using the Thermo-Calc Fortan interface is presented. The phase boundary conditions are described by a quasi-equilibrium model which uses the driving-force as an additional degree of freedom and also includes metastable interfaces. This general approach can be applied to various types of alloys for which databases are available and for an arbitrary number of alloy components and phases. The model is applied to hypereutectic aluminum casting alloys, which exhibit a rather complex solidification sequence and microstructure. Systematic variation of local solidification parameters is used to obtain a general knowledge about microstructural parameters, which can be later used in process optimization.

9:40 AM
Kinetics of Primary Crystallization Studied by Phase-Field Simulations: Pere Bruna[1]; Eloi Pineda[2]; *Daniel Crespo*[1]; [1]Universitat Politecnica de Catalunya, Dept. Fisica Aplicada, Escola Politecnica Superior de Castelldefels, Avda. del Canal Olimpic s/n, Castelldefels 08860 Spain; [2]Universitat Politecnica de Catalunya, Dept. de Fisica i Enginyeria Nuclear, ESAB, Urgell 187, Barcelona 08036 Spain

Primary crystallization of metallic glasses usually results on a high density of nanocrystallites of limited size; this fact usually leads to an improvement in the macroscopic properties of the glass. The diffusion of those species lacking or exceeding in the crystallized phase is known to stabilize the precursor phase, inducing a non-random nucleation; besides, the overlapping of the concentration profiles around neighbor growing grains reduces the growth rate (soft impingement). Although calorimetric data of these transformations was modeled by introducing empirical descriptions of soft-impingement on the Avrami framework, realistic phase-field simulations with constant diffusion coefficient cannot account for the observed experimental delays in the transformation rate. Thus, the change in the relaxation properties of the amorphous phase due to the local varying composition, usually neglected, may modify the local diffusion properties. In this work, a 3D phase-field simulation of a primary crystallization with a composition dependent diffusion is presented.

10:00 AM
2D and 3D Phase Transformations in Ternary Polymeric Membrane Systems with Variable Mobilities and Viscosity: *Bo Zhou*[1]; Adam C. Powell[1]; [1]Massachusetts Institute of Technology, Dept. of Matls. Sci. & Engrg., 77 Mass. Ave., Rm. 4-043, Cambridge, MA 02139 USA

Most commercial polymeric membranes are made from nonsolvent/solvent/polymer ternary systems by immersion precipitation. In this work, a ternary Cahn-Hilliard formulation incorporating a Flory-Huggins homogeneous free energy function is used to study the kinetics and the phase behavior of the immersion precipitation process. The Water/DMF/PVDF ternary system with a two-layer polymer-solvent/nonsolvent initial condition is used to simulate actual membrane fabrication conditions. 2D and 3D simulation results show the membrane morphology evolution during the spinodal decomposition. The simulated final morphologies show an asymmetric structure of membranes, which strongly agrees with the experimental observation. Simulations with different initial compositions show membrane morphology changes from isolated droplets to bicontinuous patterns. Furthermore, the effects of concentration-dependent polymer mobility are studied. In addition, the Navier-Stokes equations are coupled with this ternary system to model hydrodynamics with concentration-dependent viscosity in 2D and 3D. The results show that fluid flow destabilizes the top layer of membrane, with larger surface tension and smaller viscosity making the top layer more unstable.

10:20 AM Break

10:30 AM Invited
Multi-Scale Phase Field Modeling of Solute Segregation at Grain Boundaries: Ning Ma[1]; Ken R. Elder[2]; Suliman A. Dregia[1]; *Yunzhi Wang*[1]; [1]Ohio State University, Matls. Sci. & Engrg., 2041 College Rd., Columbus, OH 43210 USA; [2]Oakland University, Dept. of Physics, Rochester, MI 48309 USA

We investigate solute segregation at grain boundaries using both mesoscale and atomic scale phase field models. The mesoscale phase field model is based on gradient thermodynamics, and it differs from much previous work because it takes into account self consistently the effect of concentration gradient, spatial variation of gradient-energy coefficient and concentration dependence of solute-boundary interactions. The model predicts a sharp transition of grain boundary mobility as a function of temperature, which is related to the sharp transition of solute concentration of grain boundary as a function of temperature. The mesoscale model is, however, limited by its assumption of a uniform solute-boundary interaction potential along a boundary. The atomic scale phase field model is based on the phase field crystal model, which implements the phase field kinetic equations using atomic-resolution, time-averaged particle density as one of the field variables. The model accounts self-consistently for defect core structures at different types of grain boundaries. Different characteristics of solute distribution at different types of grain boundaries and its effect on subsequent spinodal decomposition are discussed, and results are compared with those obtained from the mesoscale phase field model.

11:00 AM Invited
Lattice Mismatch and Microstructure Evolution in Ni-Base Alloys: T. Wang[1]; J. Zhu[1]; Y. Wang[1]; S. H. Zhou[1]; Z. K. Liu[1]; *L. Q. Chen*[1]; [1]Pennsylvania State University, Matls. Sci. & Engrg., 102 Steidle Bldg., Univ. Park, PA 16802 USA

Ni-based superalloys consist of ordered intermetallic gamma-prime(Ni3Al) precipitates embedded in a disordered face-centered cubic (fcc) gamma matrix. The morphology of gamma-prime precipitates is critically dependent on the lattice parameter differences between the precipitates and matrix. This presentation will describe our recent efforts for studying the compositional dependence of lattice parameters of gamma and gamma-prime within the CMSX series of superalloys using a combination of first-principles calculations and the CALPHAD approach as well as for extending our phase-field simulations of gamma-prime precipitate microstructure evolution beyond binaries. In particular, the effect of various solute substitutions on the lattice parameter will be studied and compared with existing experimental measurements. The compositional dependence of gamma-prime precipitate morphologies and coarsening kinetics is systematically studied. Finally, the possibility of further extending the phase-field models to high-order multicomponent alloys will be discussed.

11:30 AM
A Phase-Field Model of Microstructural Evolution in Ferromagnetic Shape Memory Alloys: *Todd M. Heil*[1]; William T.

Reynolds[1]; [1]Virginia Tech, Matls. Sci. & Engrg. Dept., Ste. 302 Collegiate Sq., MC 0286, Blacksburg, VA 24061 USA

A three-dimensional computational model is employed to simulate a proper martensitic transformation and a magnetic transition in ferromagnetic shape memory alloys. The model's free energy functional is based upon phase field microelasticity and micromagnetic theories; terms are included to account for energy contributions from composition, temperature, variant boundaries, elastic strain, magnetocrystalline anisotropy, magnetic domain walls, magnetostatic potential, and external applied magnetic fields. The model tracks the microstructural and magnetic responses to applied temperature, stress, and/or magnetic fields. Model parameters are fitted to the physical properties and transformation temperatures from a series of ferromagnetic shape memory alloys in the Ni-Fe-Ga system. Magnetization and microstructural features predicted by the computational model are compared with corresponding data obtained from the Ni-Fe-Ga alloys to test the validity of the model.

11:50 AM

Simulation of Cooperative Growth of Pearlite Using Multi-Phase Field Method: *Katsumi Nakajima*[1]; Markus Apel[2]; Ingo Steinbach[2]; [1]JFE Steel Corporation, Steel Rsch. Lab., 1 Kokan-cho, Fukuyama, Hiroshima 721-8510 Japan; [2]RWTH-Aachen, Access e.V., Intzestr. 5, Aachen D-52072 Germany

The phase field method has proved to be a useful numerical tool to calculate the lamellar microstructure during eutectic solidification process. In this paper, this method is applied to eutectoid transformation in solid state. A cooperative growth of pearlite is simulated for eutectoid steel by using multi-phase field model coupled with diffusion equation, taking into consideration the diffusion of carbon not only in γ-phase, but also in α-phase. A stable lamellar spacing is estimated in conditions of some undercoolings and compared with experimental results from literature and analytical models.

12:10 PM

Phase Transformations and Microstructure Evolutions in Small Confined Systems: *Yongmei M. Jin*[1]; Yu U. Wang[2]; Armen G. Khachaturyan[1]; [1]Rutgers University, Ceram. & Matls. Engrg., 607 Taylor Rd., Piscataway, NJ 08854 USA; [2]Virginia Tech, Matls. Sci. & Engrg., Blacksburg, VA 24061 USA

Novel microstructures formed in finite volumes during decomposition, ordering and martensitic transformation in thin films, precipitate particles and polycrystal grains have been investigated by using Phase Field Microelasticity model and computer simulation. It is found that the effect of free surfaces on the micromechanics of the ordering producing L10 tetragonal phase domains in free-standing thin films changes the morphology of the domain microstructures and the structure-sensitive physical properties with respect to those in bulk. The mechanism of formation of highly dense twin-related hexagonal microdomains in non-stoichiometric Al-Mg spinel providing extraordinary hardness is investigated. It is shown that the microstructure is formed due to the isostructural spinodal decomposition into two cubic phases followed by the cubic-hexagonal transformation in small Al-rich precipitates and presumably is responsible for the advanced mechanical properties of this material. The effect of finite-sized grains of a polycrystalline body on the morphology of self-accommodating multi-variant martensitic microstructure is investigated. It is shown that the elastic grain coupling influences the thermodynamics and microstructure. The long-range elastic interaction and mechanical confinement play the key role in all these microstructure formations.

General Abstract Session: Mechanical Behavior—Quasi-Static Loading

Sponsored by: TMS

Program Organizers: Thomas R. Bieler, Michigan State University, Department of Chemical Engineering and Materials Science, East Lansing, MI 48824-1226 USA; John J. Chen, University of Auckland, Department of Chemical & Materials Engineering, Auckland 00160 New Zealand; James C. Earthman, University of California, Department of Chemical and Materials Science, Irvine, CA 92697-2575 USA

Thursday AM — Room: 2006
February 17, 2005 — Location: Moscone West Convention Center

Session Chair: Peter N. Kalu, FAMU-FSU College of Engineering, Mechl. Engrg., Tallahassee, FL 32310 USA

8:30 AM

The Room Temperature Ductility of Molybdenum with Spinel ($MgAl_2O_4$) Particles: *Joachim H. Schneibel*[1]; [1]Oak Ridge National Laboratory, Metals & Ceram. Div., PO Box 2008, Oak Ridge, TN 37831-6115 USA

In 1967, D. M. Scruggs published a patent on the improved room temperature ductility of Mo-spinel (Mo-$MgAl_2O_4$; Mo-$NiAl_2O_4$), as compared to nominally pure Mo. To verify this effect, molybdenum specimens containing 0, 5, 10, and 15 vol. % $MgAl_2O_4$ spinel powder were processed by powder metallurgy. Room temperature tensile tests were performed at different strain rates. The measured ductility values showed substantial scatter. Regardless of the spinel volume fraction, the ductility increased with decreasing fraction of intergranular fracture. The spinel ductilization effect, if it exists, was therefore overwhelmed by variations in intergranular strength. However, the fracture surface of one spinel-containing specimen showed local evidence for substantial ductility. In order to verify the spinel ductilization effect, work is in progress to minimize intergranular fracture, and thus the scatter in the ductility values, by controlling the trace element concentrations. This work was sponsored by the Office of Fossil Energy, Advanced Research Materials (ARM) Program, U.S. Department of Energy, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory managed by UT-Battelle, LLC.

9:00 AM

Deformation Behavior of Coarse Grained and Ultrafine Grained 5083 Al At 77 K and 298 K: *Kyung-Tae Park*[1]; Jun-Hwan Park[1]; Yong-Shin Lee[2]; Won-Jong Nam[3]; [1]Hanbat National University, Div. of Advd. Matls. Sci. & Engrg., San 16-1, Dukmyung-Dong, Yuseong-Gu, Taejon 305-719 S. Korea; [2]Kookmin University, Sch. of Mechl. & Auto. Engrg., 861-1, Chongneung-Dong, Songbuk-Gu, Seoul 136-702 S. Korea; [3]Kookmin University, Sch. of Advd. Matls. Engrg., 861-1, Chongneung-Dong, Songbuk-Gu, Seoul 136-702 S. Korea

Compression tests were conducted on ultrafine grained (UFG) 5083 Al alloy processed by ECAP and its coarse grained(CG)counterpart at 77 K and 298 K. Deformation of the CG alloy was dominated by the stage II and III hardening at 77 K and 298 K, respectively. The microstructure of the CG alloy deformed at 298 K consisted of well-defined dislocation cells but the blurred ill-defined cells were formed at 77 K. By contrast, the UFG alloy exhibited the elastic-near perfect plastic behavior at both temperatures. No dislocation cells were formed in the UFG alloy. Instead, localized shear bands were formed at the onset of plastic deformation at both temperatures. Based on the above findings, the effect of the grain size and temperature on the deformation mode of the alloy was analyzed.

9:30 AM

Low Temperature Creep Anomalies in Titanium Aluminum Alloys: *M. C. Brandes*[1]; M. J. Mills[1]; [1]Ohio State University, Dept. of Matls. Sci. & Engrg., 477 Watts Hall, 2041 College Rd., Columbus, OH 43210 USA

In recent studies, several creep related anomalies, particularly a marked recovery of strain hardening ensuing creep deformation at ambient temperature, were documented in metallic Ti-Al alloys. These were observed in specimens that had been loaded in compression at stresses less than the yield stresses of the materials, crept to a given level of plastic strain, unloaded, naturally aged for a period of days, and reloaded at the initial stress levels. Unexpectedly, the instantaneous strain rate upon reload was found to be higher, orders of magnitude in some cases, than that prior to the initial unload. This work presents the most current observations of the variations in the recovery re-

sponses of two Ti-6 wt% Al alloys with respect to time spent in the unloaded state, exposure temperature, accumulated plastic strain, loading geometry, and microstructure, proposes thermally activated, dislocation level recovery processes that give rise to the effect, and details planned experiments and analyses that will allow for the characterization of both the phenomenology and mechanisms of the behavior.

10:00 AM Break

10:20 AM
Effects of Initial Powder Size on the Mechanical Properties and Microstructure of As-Extruded GRCop-84: *Chika L. Okoro*[1]; Peter N. Kalu[1]; David L. Ellis[2]; [1]FAMU-FSU College of Engineering, Mechl. Engrg., Tallahassee, FL 32310 USA; [2]NASA Glenn Research Center, 21000 Brookpark Rd., Cleveland, OH 44135 USA

GRCop-84 is a ternary Cu-Cr-Nb alloy having approximately 8 at% Cr and 4 at% Nb. This work focuses on characterizing the effect of varying starting powder size on the microstructural evolution and mechanical properties of as-extruded GRCop-84. Tensile tests and constant load creep tests were performed on extrusions of four powder meshes: +140 mesh (>105 •m powder size), -140 mesh (• 105 •m), -140/+270 mesh (53 - 105 •m), and -270 mesh (•53 •m). Samples were tested in tension at room temperature and at 500ºC (932°F). Creep tests were performed under vacuum at 500ºC (932°F) using a stress of 111 MPa (16.1 ksi). The fracture surfaces of selected samples from both tests were studied using a Scanning Electron Microscope (SEM). Both optical microscopy and SEM analysis were used to characterize changes within the microstructure of the as-extruded materials due to the powder size variation.

10:50 AM
The Effect of Flash Annealing on the Mechanical and Electrical Properties of Previously Used AM2 Mats Composed of Al 6061-T6: *N. Aizpuru*[1]; D. Le[1]; J. McDonald[1]; L. McLennan[1]; S. Tewfik[1]; E. W. Lee[2]; D. Piatowski[3]; J. Foyos[1]; J. Ogren[1]; J. McLennan[1]; O. S. Es-Said[1]; [1]National Science Foundation, Loyola Marymount University, Rsch. Experience for Undergrads. Prog., Mechl. Engrg. Dept., Los Angles, CA 90045-8145 USA; [2]Naval Air Systems Command, Naval Air Warfare Ctr., Patuxent River, MD 20670-1908 USA; [3]Naval Air Systems Command, Naval Air Warfare Ctr. Aircraft Div., Lakehurst, NJ 08733 USA

Used AM2 mats (aircraft landing platforms) composed of Aluminum 6061-T6 were machined into tensile and conductivity bars. Samples were then subjected to five different temperatures: 315.6, 371.1, 426.7, 482.2 and 537.8°C (600, 700, 800, 900 and 1000°F), seven different time intervals (10, 20, 30, 70, 90, 120 and 150 seconds), and eight different exposure times (1, 2, 3, 5, 7, 10, 15 ad 20 times). The ultimate strength, yield strength, and percent elongation of the samples were determined. Conductivity and hardness tests were also performed to assess the effect of thermal exposure. Used AM2 mats are available in large quantities. It would be economical if they could be used by modern aircraft with vertical take off and landing (VTOL) capabilities that expose the mats to high temperature gaseous exhausts. The objective of this work is to evaluate the mechanical properties of the mats after several simulated take off and landing exposures. These exposures are simulated by flash annealing samples taken from the AM2 mats. Another set of AM2 mats were subjected to takeoff and landing tests performed by aircraft with Vertical Takeoff and Landing (VTOL) capabilities. The hot exhaust gases from these aircraft caused discolorations on the mat surfaces. Samples were selected radially out from the heat-affected region to examine the change of mechanical and electrical properties as a function of distance from these regions and discoloration. All samples were tested for their tensile properties as well as their conductivity (IACS %) and hardness (15-T) scale. All results were plotted according to their position from an arbitrary origin common to each of the mats.

Magnesium Technology 2005: Corrosion and Surface Finishing - Magnesium Alloys

Sponsored by: Light Metals Division, International Magnesium Association, LMD-Magnesium Committee
Program Organizers: Ramaswami Neelameggham, US Magnesium LLC, Salt Lake City, UT 84116 USA; Howard I. Kaplan, US Magnesium LLC, Salt Lake City, UT 84116 USA

Thursday AM Room: 2004
February 17, 2005 Location: Moscone West Convention Center

Session Chairs: Per Bakke, Hydro Aluminium Hycast AS, Porsgrunn 3907 Norway; Naiyi Li, Ford Motor Co, Ann Arbor, MI 48103 USA

8:30 AM
Corrosion Properties of Secondary AZ91 Alloys: *Carsten Blawert*[1]; Emma Morales[1]; Wolfgang Dietzel[1]; Norbert Hort[1]; Karl Ulrich Kainer[1]; Christiane Scharf[2]; Andre Ditze[2]; Frank Endres[2]; [1]GKSS Forschungszentrum Geesthacht GmbH, Ctr. for Mg Tech., Max-Planck-Str. 1, Geesthacht 21502 Germany; [2]TU Clausthal, Inst. für Metallurgie, Robert-Koch-Str. 42, Clausthal-Zellerfeld 38678 Germany

The corrosion properties of AZ91 alloys are determined by the amount of impurities, enriching in the alloy during the recycling process. However within reasonable costs the recycling of Mg scrap metal results only in AZ91B quality and respectively poor corrosion behaviour can be expected. This influence on the corrosion resistance was studied by controlled additions of Fe, Ni, Cu, and Si to AZ91D alloy. The corrosion properties of the gravity permanent mould castings were studied by various corrosion tests and correlated to the observed microstructure and phase composition. Most of the impurities were found as or in intermetallic phases. The influence on the corrosion resistance was found to be depending on the solidification behaviour of the particular intermetallic phase. Altogether the corrosion test results indicate a much higher tolerance against the impurities than expected and effects on the possible use of secondary AZ91 alloys are discussed.

8:50 AM
Intermetallic Morphology Development in AM60 Alloy: *Christopher Patrick Corby*[1]; Nigel Jeffrie Ricketts[2]; Ma Qian[3]; John Andrew Taylor[1]; [1]University of Queensland, CRC for Cast Metals Mfg., Div. of Matls., Sch. of Engrg., St. Lucia, Brisbane, QLD 4072 Australia; [2]CRC for Cast Metals Manufacturing, CSIRO Mfg. & Infrastruct. Tech., 2643 Moggill Rd., Pullenvale, QLD 4069 Australia; [3]Brunel University, Brunel Ctr. for Advd. Solidification Tech., Uxbridge, Middlesex UB8 3PH UK

It has been established that entrapped Al-Mn-Fe intermetallics can act as microgalvanic cathodes in magnesium alloys. Many studies present evidence suggesting these particles are Al8(Mn,Fe)5 or at least Al-Mn rich. However, the morphological development of these particles has not been documented before. This study investigates the development of these Al-Mn-Fe phases and presents evidence suggesting that two types of particle form in an AM60 melt. There are nearly spherical Al8(Mn,Fe)5 particles which sink in the melt and collect as sludge, and there is an Al-Mn rich phase, which may also be Al8(Mn,Fe)5, that grows over long holding times into floating intermetallic particles. These suspended particles are quite different in appearance to, and have lower Fe contents than the sludge particles. They initially form as faceted particles and then grow into complex floral structures after many hours holding time. These floral structures develop with more branching when holding temperature is higher.

9:10 AM
EIS Study of Corrosion Behaviour of AZ91 and AM50 Alloys: *Emmanuel Rocca*[1]; *Joseph Hazan*[1]; [1]University Henri Poincaré, LCSM UMR7555, BP239, Vandoeuvre-Les-Nancy 54506 France

The corrosion and electrochemical behaviour of AZ91 and AM50 magnesium alloys in aerated, unbuffered ASTM D13847 water have been investigated using steady-state polarization curves and mainly electrochemical impedance spectroscopy. Two relatively well separated capacitive loops can be generally observed in the complex plot for the stationary electrodes used which indicate that some protective behaviour is reached due to a film formed on the surface of the alloys. This passivation is stimulated by a pH increase accompanied by an increase of potential resulting in an anodic control. The second time constant seems related to a diffusion process through the film. So the corrosion resistance of the alloy containing a higher content of aluminium (AZ91) is better in comparison to the other alloy studied

(AM50). The RHF resistance value is a good parameter to determine more accurately the corrosion rates for magnesium alloys.

9:30 AM
Evaluation of Corrosion Protection Methods for Magnesium Alloys in Automotive Applications: *Gregory T. Bretz*[1]; Patrick J. Blanchard[1]; David J. Hill[1]; Robert C. McCune[1]; [1]Ford Motor Company, Rsch. & Advd. Engrg., PO Box 2053, MD3135 SRL, Dearborn, MI 48121 USA

Magnesium alloys are susceptible to galvanic corrosion. Consequently, it is often necessary to apply coatings to components for isolation purposes. However, previous publications suggest the effectiveness of commercial coatings can vary widely. Therefore, a screening study was performed to evaluate pre-treatment and coating systems currently available for use within the automotive industry. This paper focuses on a selection of conversion and anodized coatings. In many instances, these coatings were used in conjunction with either powder coat or an electro-coat to assess the additional protection offered by a supplemental barrier. Results from the study include SEM micrographs to highlight coating thickness and morphology. A correlation is then made between the SEM analysis and performance of specimens subjected to accelerated corrosion testing. Finally, sample sections are examined to show the nature of the corrosive attack, and highlight the robustness and physical protection offered by respective coating systems.

9:50 AM Break

10:05 AM
Corrosion Inhibition of Magnesium Alloys in Coolants: Guangling Song[1]; *David H. StJohn*[1]; [1]University of Queensland, Matls., St. Lucia, Brisbane 4071 Australia

A number of magnesium alloys show promise as engine block materials. However, corrosion of magnesium alloy engine components by coolant is an important issue in the automotive industry. This paper shows that the corrosion rate of magnesium was increased by dilution and contamination of ethylene glycol. Fortunately, the corrosion of magnesium in ethylene glycol can be effectively inhibited by addition of fluorides. This finding was further verified by assessing the corrosion performance of AZ91D and a recently developed engine block magnesium alloy AM-SC1 in several commercial coolants. Generally speaking, the tested commercial coolants were corrosive to the magnesium alloys in terms of general and galvanic corrosion, but an organic-acid based long-life coolant appeared to be less corrosive than a traditional coolant. It was found that both general and galvanic corrosion rates were significantly decreased by addition of KF, and there were no evident side effects on the other engine block materials, such as copper, solder, brass, steel and aluminium alloys, in terms of their corrosion performance. The ASTM D 1384 test further confirmed these results and suggested that Toyota long life coolant with a KF addition is a promising coolant for magnesium engine blocks.

10:25 AM
Characterization of Die Skin Structure and its Effects on the Corrosion Properties of the Hot-Chamber Die Casting AZ91D Thin Plate: *Jun-Yen Uan*[1]; Bing-Lung Yu[1]; [1]National Chung Hsing University, Dept. of Matls. Engrg., 250 Kuo Kuang Rd., Taichung 402 Taiwan

The corrosion of hot-chamber die cast AZ91D thin plates was investigated with reference to their microstructures, to elucidate the role of die chill skin in the corrosion. At pH 2.7 in a chloride solution, the sample with die skin corrodes at 200~250 miles per year (mpy), whereas the sample without the die skin exhibits a corrosion rate of 100~150 mpy. The two kinds of samples have similar Ecorr values of -1.45 V. However, the mean Icorr value of the sample with die skin is 150~250 ìA/cm2, whereas that of the sample without die skin is only 40~60 ìA/cm2. Immersion tests and polarization experiments reveal the inferior corrosion performance of the specimen with the die skin on the surface. The die skin structure was explored. The corrosion performance of the hot-chamber die cast thin plate with die skin is closely related to the morphology and distribution of the Al12Mg17 â phase in the matrix.

10:45 AM
Microstructure and Wear Characteristic of Laser Clad Al-12% Si, Al-30% Si and ALSI/WC on AS21 Magnesium Alloy: *Meity Natasya Mandagie*[1]; Milan Brandt[1]; Yvonne Durandet[1]; Mahnaz Jahedi[2]; [1]Swinburne University of Technology, IRIS, PO Box 218, Hawthorn, Melbourne, Victoria 3123 Australia; [2]CSIRO, Mfg. & Infrastruct. Tech., Locked Bag 9, Preston, Melbourne, Victoria 3072 Australia

Although magnesium alloys possess a set of desirable properties such as low specific weight and high specific strength that make them attractive to automotive and aerospace industries, they have poor wear and corrosion resistance compared to that of steel or aluminium alloys. This is due to their relatively low surface hardness and high chemical affinity for numerous elements. This study investigates the microstructure and wear characteristics of clad layers made of Al-12% Si, Al-30%Si, and a mixture of Al-12%Si (40%) and WC (60%). The claddings were deposited on creep resistant AS21 magnesium alloys using a high power Nd: YAG laser. The results indicate that the clad layers have better wear resistance than the substrate.

11:05 AM
The Electropolishing and Anodic Coating of AZ31 Magnesium Alloy in Anhydrous Electrolyte: *Qun Zhao*[1]; Yuanfu Zhou[1]; Ying Zhang[1]; Chunfang Zhao[1]; Yonghen Guo[1]; Xianghui Cang[1]; [1]Zhengzhou Research Institute of Chalco, Aluminum Corporation of China Limited, No.82, Jiyuan Rd., Shangjie Dist., Zhengzhou, Henan 450041 China

The metallic shining surface of AZ31 magnesium alloy strip was obtained by electropolishing process in anhydrous electrolyte, in which a thick phosphate chemical conversion coating was formed by anodic polarization. The influence of water concentration on the properties of electrolyte and the electrochemical process were investigated at the same time. The microstructure of the bright surface and anodic oxidizing coating were observed using SEM and XRD.

11:25 AM
Corrosion Protection and Repassivation After the Deformation of Magnesium Alloys Coated With a Protective Magnesium Fluoride Layer: Friedrich Wilhelm Bach[1]; *Thomas Hassel*[1]; Christian Krause[1]; Peter Wilk[1]; [1]University of Hannover, Dept. of Matls. Sci., Schoenebecker Allee 2, PZH, Garbsen, Low Saxonia D-30823 Germany

The development of a biodegradable, cardiovascular implant (stent) made from a resorbable magnesium alloy demands an accurately defined degradation profile. The corrosion protection of the stent for the first 4-6 weeks after implantation is only obtainable by usage of a surface protective coating. During this time the implant is able to grow into the vessel. After the steady solution of the coating the base material is resorbed by a normal corrosion process in chloride media. During the implantation the material has to tolerate partial deformations. The influence of the induced micro-cracks during the deformation process has been analysed in a 4-point bending test combined with an electrochemical corrosion test. The material system consists of a Mg(Ca<1wt%)-alloy and a dense MgF2-coating. The coating process is based on the conversion of the natural layer by a treatment with hydrofluoric acid. The specimens show micro-cracks after the deformation but no increased corrosion activity. The measurement of the corrosion current indicates a repassivation of the surface. Detailed EDX and REM analyses prove the regeneration of Mg(OH)2/MgO on the crack ground.

11:45 AM
Mg2Si Coating Technology on Magnesium Alloys to Improve Corrosion and Wear Resistance: *Takashi Yamaguchi*[1]; Katsuyoshi Kondoh[2]; Tadashi Serikawa[2]; Momoko Henmi[2]; Hideki Oginuma[2]; [1]Gifu Prefectural Science and Technology Promotion Center, 4-179-1, Sue-Cho, Kakamigahara-City, Gifu pref. Japan; [2]University of Tokyo, Rsch. Ctr. for Advd. Sci. & Tech., 4-6-1 Komaba, Meguro-ku, Tokyo Japan

Magnesium silicide (Mg2Si) bulky material has a possibility to improve the surface function of light metals such as magnesium and aluminum alloys due to its superior corrosion resistance to the conventional stainless steel and high mechanical properties. In this study, Mg2Si thin film coated on AZ31 magnesium alloys by using a high frequency sputtering method was examined. Salt spray test to evaluate the corrosion resistance indicated that AZ31 substrate with Mg2Si coating was hardly damaged after 240h. On the other hand, non-treated one was corroded in only 1h. Concerning the wear resistance under oil lubricant test, a friction coefficient, ¯¬ of the AZ31 alloy with Mg2Si film is remarkably stable in employing S35C steel as a counter specimen. In the combination of AZ31 alloy disc and S35C pin specimens, seizure and sticking phenomena occurred and ¦Ì value suddenly increased. Accordingly, Mg2Si coating technology is a suitable surface modification processing to improve corrosion and wear resistance of magnesium alloys.

Materials Issues for Advanced Nuclear Systems: Materials Compatibility

Sponsored by: Structural Materials Division, SMD-Nuclear Materials Committee-(Jt. ASM-MSCTS)
Program Organizers: Robert J. Hanrahan, Los Alamos National Laboratory, Los Alamos, NM 87545 USA; Sean M. McDeavitt, Argonne National Laboratory, Chemical Technology Division Materials Development Section, Argonne, IL 60439-4837 USA

Thursday AM Room: 3012
February 17, 2005 Location: Moscone West Convention Center

Session Chairs: Sean M. McDeavitt, Purdue University, Nucl. Engrg., Purdue, IN USA; Robert J. Hanrahan, Los Alamos National Laboratory, NNSA, Washington, DC 22209 USA

8:30 AM
SiC/SiC for Advanced Reactors: *Russell H. Jones*[1]; [1]Pacific Northwest National Laboratory, Matls. Sci. Div., PO Box 999, Richland, WA 99354 USA

Composite materials have the potential for their properties to be tailored to specific applications by engineering the combination of fibers and matrices. Ceramic matrix composites are attractive because of their excellent high-temperature properties and corrosion resistance. In particular, ceramic composites made from silicon carbide fibers and silicon carbide matrices (SiCf/SiC) are promising for nuclear applications because of the radiation resistance of the b phase of SiC, their excellent high-temperature fracture, creep, corrosion and thermal shock resistance. The b phase of SiC has been shown by numerous studies to have a saturation swelling value of about 0.1 to 0.2% at 800 to 1000 C. This suggests that composites of SiC/SiC have the potential for excellent radiation stability. The continuous fiber architecture, coupled with engineered interfaces between the fiber and matrix, provide excellent fracture properties and fracture toughness values on the order of 25 MPa m 1/2. The strength and fracture toughness are independent of temperature up to the limit of the fiber stability. Also, these fiber/matrix microstructures impart excellent thermal shock and thermal fatigue resistance to these materials so start-up and shut-down cycles and coolant loss scenarios should not induce significant structural damage.

9:00 AM
Fuel-Cladding Compatibility in Metallic Nuclear Fuels: *Dennis D. Keiser*[1]; James I. Cole[1]; [1]Argonne National Laboratory-West, Engrg. Tech. Div., PO Box 2528, Idaho Falls, ID 83403-2528 USA

In advanced nuclear systems, the chemical compatibility of the fuel and cladding is imperative for safe operation of a reactor. Interactions between fuel and cladding during irradiation can result in the formation of strength reducing zones in the cladding and the formation of compositional zones with melting points below the anticipated operating temperatures. Therefore, it is essential to limit the interdiffusion between the fuel and cladding. To better understand the compatibility of metallic fuel and cladding, diffusion experiments were conducted at prototypic temperatures using fuel alloys and various stainless steel claddings. Additionally, diffusion experiments were performed using fuel, cladding, and materials that may act as barriers to fuel-cladding interaction (viz., V, Zr, and Ta). The various annealed diffusion couples were analyzed using scanning electron microscopy and transmission electron microscopy to investigate the kinetics of the fuel-cladding interactions and to identify the types of phases that formed. The results of these analyses will be described, along with the effectiveness of the barrier materials at impeding interdiffusion between the fuel and cladding alloys.

9:30 AM
Effects of Irradiation on Materials for Advanced Gas Cooled Reactors: *Wolfgang Hoffelner*[1]; Manuel Alexandre Pouchon[1]; Jiachao Chen[1]; [1]Paul Scherrer Institute, Nuclear Energy & Safety, Villigen PSI CH-5232 Switzerland

Gas cooled reactors are considered as future plants for sustainable co-generation of electric energy and heat (Generation IV initiative). For advanced plant designs high temperature materials like ODS or intermetallics become important. The interaction of irradiation induced defects, transmutation products and eventual grain boundary voids with diffusion controlled processes like creep are life-limiting factors. Samples of the ferritic ODS alloy PM 2000 (Plansee) and of a lamellar, W-containing titanium aluminide (ABB-2) were subjected to He-implantation, in order to investigate changes in microstructure and swelling behaviour of the material. The implantations were performed at different temperatures (room temperature up to 1000 C). The ODS material was irradiated with 1.5 MeV under four different angles to get a homogeneous damage profile. The investigated damage range was 0.25 to 2 dpa. Swelling was measured with atomic force microscope (AFM). Irradiation of the TiAl was done at an energy of up to 24 MeV. Microstructural damage analysis was performed with TEM. The results are discussed with respect to expected changes of mechanical properties.

10:00 AM Break

10:20 AM
Selection of a Canister Crucible Material for the Mobile Melt-Dilute Process: *Brian Robert Westphal*[1]; Dave A. Sell[1]; Dennis D. Keiser[1]; [1]Argonne National Laboratory, PO Box 2528, Idaho Falls, ID 83403-2528 USA

As part of the mobile melt-dilute project for the processing of spent nuclear fuel in the Former Soviet Union (FSU), the selection of a canister crucible is of considerable importance for containment of a molten fuel matrix. During the process, a highly enriched aluminum-uranium fuel is diluted isotopically to satisfy proliferation concerns. The crucible material must sustain the high temperature dilution operation as well as be compatible with either storage or subsequent processing schemes. In addition, the crucible material must be readily available in the FSU and easily fabricated into a canister design. A materials testing program was initiated to identify the compatibility of potential crucible materials with the mobile melt-dilute process. Following a series of preliminary screening tests, scale-up testing was performed with the crucible material of choice and an aluminum-uranium feed. Results from the testing program are presented along with a justification for the material selection.

10:50 AM
Systematical Investigation on the Luminescence Enhancement of PbWO4 Crystals by Doping and Annealing: *Yanlin Huang*[1]; [1]Zhong Yuan Institute of Technology, Dept. of Mechl. Engrg., 41 Zhongyuan W. Rd., Zhengzhou, Henan 450007 China

PbWO4 crystal has been chosen for a scintillating detector at the Large Hadron Collider (LHC) in CERN due to its high density, short radiation length and fast decay time. Extensive investigations have been done around the world to improve the scintillation performance by annealing treatment and aliavalent ion doping in the crystals. The works in this report are focused on the enhancement of light yield in PbWO4 crystals by doping and annealing, and excellent scintillation performance still are kept for this material. The doping ions in the crystal include monovalent ions, trivalent ions and co-doping between different aliavalent ions. Many results were first report in the material. Meanwhile, the annealing mechanism and aliavalent ion doping mechanism from viewpoint of microstructure were also discussed. Besides, these results reveal also that PWO might have potential use in the PET material, even in the optoelectronic application.

11:20 AM
Oxide Layers on the High Cr Steels After SCW Corrosion: *Jinsung Jang*[1]; Chang Hee Han[1]; Yong Sun Yi[1]; Seong Sik Hwang[1]; Yongbok Lee[2]; [1]KAERI, Nucl. Matl. Tech. Dvlp. Div., 150 Dukjin-dong, Yuseong-gu, Daejeon 305-353 S. Korea; [2]KRISS, Ctr. for CMR Matls., 1 Doryong-dong, Yuseong-gu, Daejeon 305-340 S. Korea

Among the candidate materials for Generation IV SCWR (Supercritical Water-cooled Reactor) four high Cr steels and one Fe-based O.D.S alloy specimens were investigated. After the SCW corrosion tests in the temperature from 400 to 627 C under 25 MPa and the weight change measurement, the oxide layers were analyzed using a grazing incidence X.R.D, S.E.M and T.E.M. Cross sectional view of the oxide scale on the 9Cr steel specimen after the corrosion test was found to consist of three distinctive layers. The outermost layer with about a 35 micron thickness after 200 hr at 627 C was identified to be Fe3O4, and the intermediate layer of about 25 micron thickness was revealed to be Cr partitioned (Fe,Cr)3O4. The innermost layer next to the matrix was the internally oxidized zone. Oxygen atoms apparently diffused along the grain boundaries and the lath boundaries, forming oxide phase of (Fe,Cr)3O4 or (Fe,Cr)2O3 along the boundaries.

Micromechanics of Advanced Materials II (Symposium in Honor of James C.M. Li's 80th Birthday): Thin Films and Multilayers

Sponsored by: Structural Materials Division, ASM International: Materials Science Critical Technology Sector, SMD-Mechanical Behavior of Materials-(Jt. ASM-MSCTS)

Program Organizers: Fuqian Yang, University of Kentucky, Department of Chemical and Materials Engineering, Lexington, KY 40506 USA; C. C. Chau, Pactiv Corporation, Canandaigua Technology Center, Canandaigua, NY 14424 USA; Sung Nee George Chu, Multiplex Inc, South Plainfield, NJ 07080 USA; M. Ashraf Imam, Naval Research Laboratory, Materials Science & Technology Division, Washington, DC 20375-5343 USA; Teh-Ming Kung, Eastman Kodak Company, Rochester, NY 14650 USA; Peter K. Liaw, University of Tennessee, Materials Science and Engineering, Knoxville, TN 37996-2200 USA; B. B. Rath, Naval Research Laboratory, Materials Science and Component Technology Directorate, Washington, DC 20375-5341 USA

Thursday AM Room: 3000
February 17, 2005 Location: Moscone West Convention Center

Session Chair: H. Y. Yu, US Army International Technology Center - Pacific, Asian Rsch. Office, Minato-Ku, Tokyo 106-0032 Japan

8:30 AM Invited
Influence of Cathode Oxide Films on Copper Nucleation During Electrodeposition: Hyunku Chang[1]; Byung-Hak Choe[2]; *Jong K. Lee*[3]; [1]Sungkyunkwan University, Sch. of Applied Matls. Engrg., Suwon 440-746 Korea; [2]Kangnung National University, Dept. of Metallurgl. Engrg., Kangnung 210-702 Korea; [3]Michigan Technological University, Dept. of Matl. Sci. & Engrg., Houghton, MI 49931 USA

Copper electrodeposition has an important industrial role because of various interconnects used in microelectronic devices. A typical deposition process utilizes a titanium cathode as the finished copper foil is easily separable from the thin passive TiO2 oxide layer, 2 to 3 nm thick, of the cathode. In this work, the effect of the oxide layer on copper nucleation was studied through both "ex-situ" and "in-situ" nano-scratch tests. In the case of ex-situ tests, an MTS-XP indenter was employed to induce scratches onto the cathode surface as a function of a load up to 0.6 Newtons. For "in-situ" experiments, the cathode surface was, while immersed in the electrolyte cell, scratched with a blade. In both cases, higher copper cluster densities, by a factor of 10 to 100, were observed along the scratch lines, indicating that dislocations were favored nucleation sites for copper deposition. A pipe tunneling mechanism along dislocation cores was proposed to account for the enhanced nucleation rate. With both a reduced energy barrier and a reduced barrier thickness, a dislocation line is considered to be a high electron tunneling path within an oxide layer of a large band energy gap.

8:55 AM Invited
Microbridge Testing of Thin Films: *Tong-Yi Zhang*[1]; [1]Hong Kong University of Science and Technology, Dept. of Mechl. Engrg., Clear Water Bay, Kowloon Hong Kong

In the present work, we summarize the novel microbridge testing method for thin films including single-layer, bilayer, and trilayer thin films. The samples for microbridge tests were prepared with the microelectromechanical fabrication technique such that they were easy to be handled with. The microbridge test was conducted with a load and displacement sensing nanoindenter system equipped with a microwedge probe. In mechanics analysis of the microbridge deflection versus load under large deformation, we modeled the substrate deformation with three coupled springs and considered residual stress in each layer, thereby resulting in a closed-form formula. The microbridge testing method allows us to simultaneously evaluate the Young's modulus, residual stress and bending fracture strength of single-layer films from an experimental load-deflection curve. For bilayer and trilayer films, the analysis shows that bending of a bilayer or trilayer beam is equivalent to the bending of a single-layer beam with an equivalen t bending stiffness, a residual force and a residual moment. Therefore, the closed formula is able to simultaneously evaluate the equivalent bending stiffness, the residual force and the bending strength from the microbridge test. In general, one can estimate the Young's modulus and residual stress in one layer if the corresponding values in the other n-1 layers are known. Alternately, we may first take the slope of a load-deflection curve under small deformation, which gives the relationship between the bending stiffness and the residual force of a bilayer or a trilayer microbridge. Then, using this relationship, we were able to evaluate the Young's modulus of two kinds of materials composing the bilayer or trilayer film and the average residual stress of the film simultaneously. All the theoretical formulas have been verified experimentally on single-layer, bilayer and trilayer films.

9:20 AM Invited
Piezoelectric Polarization Induced Two Dimensional Electron Gases in AlGaN/GaN Heteroepitaxial Structures: An Application for Micro-Pressure Sensors: *S. N.G. Chu*[1]; F. Ren[2]; S. J. Pearton[3]; B. S. Kang[2]; S. Kim[2]; B. P. Gila[3]; C. R. Abernathy[3]; J. Lin[4]; [1]Multiplex Inc., S. Plainfield, NJ 07080 USA; [2]University of Florida, Dept. of Cheml. Engrg., Gainesville, FL 32611 USA; [3]University of Florida, Matls. Sci. & Engrg., Gainesville, FL 32611 USA; [4]University of Florida, Electl. Engrg., Gainesville, FL 32611 USA

The wurtzite group-III nitrides exhibit piezoelectric polarization along their c-axis. Differential piezoelectric and spontaneous polarizations in strained AlGaN/GaN heterostructure grown on [0001] sapphire substrates induce two-dimensional electron gas (2DEG) at the AlGaN/GaN hetero-interface. AlGaN/GaN high electron mobility transistors (HEMT) based on electrical polarization induced 2DEG are therefore sensitive to the applied stresses. We demonstrate the feasibility of fabrication of such devices and their response to the applied stresses. Since these devices can be made onto small thin GaN membranes by removing locally the sapphire substrate using the present state-of-the-art micro-fabrication technologies, pressure sensors in the micrometer scale are possible. AlGaN/GaN/sapphire material system is ideal for high temperature applications as well as for hush chemically environments. It can also be a potential micro-sensor for medical implant applications. A detailed theoretical analysis of the dependence of trans-conductance of HEMT device on the applied stresses is provided to give insight to the stress response mechanism of the device.

9:45 AM Invited
Layer Piling Effect on Mechanical Properties of Triple-Layer Disc: *Der-Ray Huang*[1]; Tzuan-Ren Jeng[1]; Huei-Wen Yang[1]; [1]Industrial Technology Research Institute, Opto-Elect. & Sys. Labs., Chutung, Hsinchu Taiwan

To approach higher storage density, multi-layer optical disc that fabricated by photo-polymer UV curing method has become popular subject recently. In this paper, a triple layer optical disc made by new piling method has been developed. A 0.6mm thick polycarbonate substrate with first layer data (L0) is obtained from the typical injection mold. Then a silicon film was sputtered on it as first reflection layer. For second data layer (L1), one special kind of duplication method is introduced. A stamper with L1 data pit is applied as the replication source. In the next step, an UV cured acrylic resin was dispensed and spin-coated on L0. After pressing and UV curing, the stmaper could be easily separated from L0 substrate. L1 is found to stack on the L0. AgTi film is sputtered on the top of L1 as second reflection layer. As for third data layer (L2) the process is similar to L1. AgTi film is sputtered on L2 surface as third reflection layer. After bonding with a 0.6mm dummy substrate, a triple-layered disc is obtained. The surface roughness of each layer can be measured with atomic force microscope. The first surface roughness of L0 comes from ultra precision injection molding process. The data jitter of the first layer L0 is easy to be less than 7%. However, for L1 and L2, the roughness arises from the combination of photo-polymer molecular size and layer piling effect. Thus L1 and L2 with worse data jitter are expected. And from the dish measurement, we can learn the effect of stress created from layer adhesive process. The detail experimental data of the static and dynamic measurement result will be discussed.

10:10 AM Invited
Residual Stress in DVDR: *Hsueh-Lung Cheng*[1]; Der-Ray Huang[2]; Tzuan-Ren Jeng[2]; Wen-Yih Liao[1]; Sanboh Lee[1]; [1]National Tsing Hua University, Matls. Sci. & Engrg., Hsinchu Taiwan; [2]Industrial Technology Research Institute, Opto-Elect. & Sys. Labs., Chutung, Hsinchu Taiwan

Digital Versatile Disc Recordable (DVDR) consists of dye layer, reflective layer and protective layer deposited on polycarbonate (PC) substrate of thickness 0.6mm. First, the dye layer was coated on PC substrate using a spin coater. Second, a layer of silver as a reflective layer is deposited on dye layer using a DC sputter. Third, a new PC substrate as a protective layer was bonded on the reflective layer using UV curable glue. The curvatures before and after deposition of each process were measured. The residual stresses in each layer were calculated when curvature and elastic constants of each layer are given. It is found that after the protective layer was bonded on the reflective

layer, the residual stresses in protective layer increases with increasing thickness of reflective layer. The effect of dye thickness on residual stresses is also included.

10:35 AM
Thermoelastic Bending of Multilayer Structures: *Xinzhong Zhang*[1]; J. C.M. Li[1]; [1]University of Rochester, Dept. of Mechl. Engrg., Rochester, NY 14627 USA

The bending curvature due to strain mismatch in a multilayer strip or plate structure is analysed. The analytical results are compared with finite element computations. Early results of Stoney and Timoshenko are confirmed. For multilayer plates there is a critical curvature after which bifurcation takes place, namely, the plate will bend in two curvatures. This bifurcation limit is shown also by finite element analysis. Work supported by NSF through DMR-9623808 monitored by Bruce MacDonald.

10:55 AM Break

Micromechanics of Advanced Materials II (Symposium in Honor of James C.M. Li's 80th Birthday): Shock Compression

Sponsored by: Structural Materials Division, ASM International: Materials Science Critical Technology Sector, SMD-Mechanical Behavior of Materials-(Jt. ASM-MSCTS)
Program Organizers: Fuqian Yang, University of Kentucky, Department of Chemical and Materials Engineering, Lexington, KY 40506 USA; C. C. Chau, Pactiv Corporation, Canandaigua Technology Center, Canandaigua, NY 14424 USA; Sung Nee George Chu, Multiplex Inc, South Plainfield, NJ 07080 USA; M. Ashraf Imam, Naval Research Laboratory, Materials Science & Technology Division, Washington, DC 20375-5343 USA; Teh-Ming Kung, Eastman Kodak Company, Rochester, NY 14650 USA; Peter K. Liaw, University of Tennessee, Materials Science and Engineering, Knoxville, TN 37996-2200 USA; B. B. Rath, Naval Research Laboratory, Materials Science and Component Technology Directorate, Washington, DC 20375-5341 USA

Thursday AM Room: 3000
February 17, 2005 Location: Moscone West Convention Center

Session Chair: J. C.M. Li, University of Rochester, Mechl. Engrg. Dept., Rochester, NY 14627 USA

11:00 AM Invited
Effect of Shock Compression Method on the Defect Substructure in Single Crystal Cu: *Bu Yang Cao*[1]; Marc Andre Meyers[1]; David H. Lassila[2]; Yong Bo Xu[3]; Bruce A. Remington[2]; Chongxiang Huang[3]; Matt S. Schneider[1]; Daniel H. Kalantar[2]; [1]University of California, Matls. Sci. & Engrg., 9500 Gilman Dr., UCSD 0411, La Jolla, CA 92093 USA; [2]Lawrence Livermore National Laboratory, Livermore, CA 94550 USA; [3]Chinese Academy of Sciences, Shenyang Natl. Lab. for Matls. Sci., Inst. of Metal, Shenyang, Liao Ning 110016 China

Monocrystalline copper samples with orientations of [001] and [221] were shocked at pressures ranging from 20 GPa to 60 GPa using two techniques: direct drive lasers and explosively driven flyer plates. The pulse duration for these techniques differed substantially: 2 ns for the laser experiments and 1 us for the flyer plate experiments. Defects were investigated by transmission electron microscopy and an analytical model of homogeneous dislocation nucleation is proposed. The residual microstructures were dependent on orientation and pressure. The samples shock compressed by flyer plate showed ample evidence of recrystallization and major microstructural reorganization at amplitudes of 47 GPa, whereas the laser shock compressed specimens retained shock induced microstructures up to 60 GPa. The post-shock cooling rates in laser shock compression are orders of magnitude higher than in the flyer-plate shock compression. Because the pulse duration is short in laser shock experiments, the specimens are rapidly quenched and only limited dislocation motion and post shock recovery processes occur. These differences are studied using an analytical model of thermal diffusion. This study demonstrates the unique advantage of laser shock compression in recovery experiments. Research funded by DOE and LLNL.

11:25 AM
Characterization and Modeling of Laser Induced Shock Compression of NiAl Single Crystals: *Chyi Hwang Lim*[1]; [1]Arizona State University, Mechl. & Aeros. Engrg., PO Box 876106, Tempe, AZ 85287-6106 USA

Direct drive laser irradiation tests have been performed on monocrystalline NiAl samples 150 to 300 microns thick and 5 mm in diameter. The samples were subjected to shock pressures of 10.3 GPa for the <100> loading direction and 19.4 GPa for <110> and <111> loading directions to study anisotropic material response under high strain rate deformation. Analyses of recovered samples were performed using Orientation Imaging Microscopy (OIM) revealing a region of high lattice rotation spanning a thickness of about 20 microns from the shocked surface. It was found that the magnitude of the lattice rotation measured correlates to the total number of potentially active slip systems of the {110}<001> and{100}<010> type with <001>, <011> and <111> loading axes having zero, six and nine potentially active slip systems, respectively. An incremental single crystal plasticity model was used to model NiAl behavior, including lattice rotation, for the simple case of uniaxial compression.

11:45 AM Closing Remarks: Dr. J. C.M. Li

Microstructural Processes in Irradiated Materials: Mechanical Behavior of Irradiated Materials

Sponsored by: Structural Materials Division, SMD-Nuclear Materials Committee-(Jt. ASM-MSCTS)
Program Organizers: Brian D. Wirth, University of California, Department of Nuclear Engineering, Berkeley, CA 94720-1730 USA; Charlotte S. Becquart, Ecole Nationale Superieure de Chimie de Lille, Laboratoire de Metallurgie Physique et Genie des Materiaux, Villeneuve d'Ascq cedex 59655 France; Hideki Matsui, Tohoku University, Institute for Materials Research Japan; Lance L. Snead, Oak Ridge National Laboratory, Metals and Ceramics Division, Oak Ridge, TN 37830-6138 USA

Thursday AM Room: 3011
February 17, 2005 Location: Moscone West Convention Center

Session Chairs: Hideki Matsui, Tohoku University, Inst. for Matls. Rsch. Japan; G. Robert Odette, University of California, Dept. of Matls., Santa Barbara, CA 93106 USA; Yoshitaka Matsukawa, Oak Ridge National Laboratory, Metals & Ceram., Oak Ridge, TN 37831-6138 USA

8:30 AM
Microstructural Analysis of Deformation in Neutron-Irradiated FCC Materials: *N. Hashimoto*[1]; T. S. Byun[1]; K. Farrell[1]; [1]Oak Ridge National Laboratory, Metals & Ceram. Div., PO Box 2008, Bldg. 4500S, Oak Ridge, TN 37831-6136 USA

Plastically deformed microstructures in neutron-irradiated face centered cubic (fcc) materials, copper, nickel and 316 stainless steel, were investigated by transmission electron microscopy (TEM). Particular emphasis is placed on the deformation microstructure responsible for the changes in mechanical behavior. Neutron irradiation at low temperature up to 1 displacement per atom (dpa) induced a high number density of small loops, stacking fault tetrahedra (SFT) and Frank loops, which resulted in irradiation-induced hardening. Deformation of irradiated fcc materials induced various microstructures, such as dislocation pileups, stacking faults, twins, and dislocation channels. At higher irradiation doses (0.1~12 dpa), dislocation channeling became the dominant deformation mode in fcc materials. In the 316 stainless steels irradiated to 0.1~0.8 dpa, the deformation microstructure consisted of a mixture of dislocation bands, tangles, twins, dislocation channels, and also martensite phase. Deformation-induced martensite transformation tends to occur with dislocation channeling, suggesting that localized deformation could lead to transformation of martensite at a high stress level.

8:50 AM
Direct Observation of SFT-Dislocation Interaction Process at Low Temperature: *Yoshitaka Matsukawa*[1]; Yuri N. Osetsky[1]; Roger E. Stoller[1]; Steven J. Zinkle[1]; [1]Oak Ridge National Laboratory, Metals & Ceram., PO Box 2008, Oak Ridge, TN 37831-6138 USA

The formation mechanism of localized defect-cluster-free zones (dislocation channeling) during deformation is of interest for understanding ductility reduction in neutron-irradiated metals. The stacking fault tetrahedron (SFT) is a major vacancy cluster produced by neutron irradiation in fcc metals; however, the SFT annihilation mechanism is hard to predict due to its complicated defect geometry. We

have recently reported SFT annihilation in quenched gold during TEM in-situ straining experiments at room temperature. Here we present the results at low temperature, where vacancy migration is suppressed in gold. A large SFT (¡Ö50nm) was collapsed by direct interaction with moving dislocations at 173K, in a manner similar to previously reported room temperature results. Possible mechanisms for the SFT collapse by dislocations will be discussed: the present results indicate that the vacancy migration is not a crucial factor for the SFT collapse mechanism.

9:10 AM
Understanding Radiation Hardening and the Conditions Promoting Localized Deformation in Neutron-Irradiated Copper: *Dan Edwards*[1]; Bachu N. Singh[2]; [1]Pacific Northwest National Laboratory, Matls. Struct. & Performance Grp., PO Box 999, MSIN P8-16, Richland, WA 99354 USA; [2]Risø National Laboratory, Matls. Rsch. Dept., Rosklide DK-4000 Denmark

The phenomenon of radiation hardening and plastic flow localization in the form of dislocation channels has been observed for more than 40 years in neutron irradiated materials, but a clear understanding of the processes the control these two phenomena elude us. This presentation will highlight the results of several recent experiments investigating the microstructural features that control the deformation behavior of irradiated copper. These experiments include in-situ tensile experiments studying the microstructural evolution in materials subjected simultaneously to neutron irradiation and tensile loading at 90°C, post-irradiation annealing experiments on neutron-irradiated copper, and finally a series of interrupted tensile tests on irradiated copper evaluating the strain-dependent evolution of localized deformation. These experimental results lead to the conclusion that the radiation hardened matrix becomes increasingly unable to activate dislocation sources within grain interiors and deform homogenously, instead, dislocation channels are initiated at high stress concentrations at interfaces.

9:30 AM
Microstructure of Neutron-Irradiated Iron Before and After Tensile Deformation: *Steven J. Zinkle*[1]; Bachu N. Singh[2]; [1]Oak Ridge National Laboratory, Metals & Ceram. Div., PO Box 2008, Oak Ridge, TN 37831-6138 USA; [2]Risoe National Laboratory, Matls. Rsch. Dept., Postbox 49, Roskilde DK-4000 Denmark

Tensile specimens of pure Fe were neutron irradiated at ~70 C in the HFIR and HFR test reactors to displacement dose levels of 0.0001 - 0.72 dpa. Irradiated specimens were characterized using transmission electron microscopy (TEM). Visible defect clusters were not detectable by TEM for doses below ~0.001 dpa. Both the density and average size of the dislocation loops increased with increasing dose level. Heterogeneous rafts of dislocation loops were visible for doses above ~0.2 dpa. The irradiation led to an increase in the yield stress and a decrease in the uniform elongation as a function of increasing dose. Examination of specimens after tensile deformation revealed localized deformation in the form of cleared dislocation channels. Relatively few channels were formed in the uniform elongation region of the gage section. Dislocation channels on multiple slip systems were observed in the deformation region near the fracture surface, presumably due to multiaxial stress state.

9:50 AM Break

10:20 AM
Molecular Dynamics Simulations of Dislocations Interacting with Vacancy Clusters in Face-Centered Cubic Metals: *Erik Bitzek*[1]; Daniel Weygand[1]; Peter Gumbsch[2]; [1]University of Karlsruhe, IZBS, Kaiserstr. 12, Karlsruhe 76131 Germany; [2]Fraunhofer Institut fuer Werkstoffmechanik IWM, Wöhlerstraße 11, Freiburg 79108 Germany

To study the hardening effect of vacancy clusters we performed atomistic simulations of straight edge and screw dislocation segments interacting with nano-scale voids. Static simulations with embedded atom potentials for nickel and aluminum were used to determine the obstacle strength of vacancy clusters. Molecular dynamics (MD) simulations were performed to study the dynamics of the dislocation - vacancy interaction. Depending on the temperature, the stress required for the approaching dislocation to pass the obstacles can be significantly lower compared to the static simulations. For the low temperature regime this dynamical effect can be attributed to the dislocation inertia. To asses the importance of dynamical effects for various dislocation - obstacle configurations, inertial effects were implemented in a discrete dislocation dynamics (DDD) simulation. With the required parameters (dislocation mass, drag coefficient and obstacle strength) determined from MD simulations, the DDD model reproduced the atomistic results of the dislocation - void interaction.

10:40 AM
Dynamics of Edge Dislocation Interaction with Self-Interstitial Clusters in Iron: Zhouwen Rong[1]; *David J. Bacon*[1]; Yuri N. Osetsky[2]; [1]University of Liverpool, Dept. of Engrg., Brownlow Hill, Liverpool L69 3GH UK; [2]Oak Ridge National Laboratory, Computer Scis. & Math. Div., PO Box 2008, Oak Ridge, TN 37831-6158 USA

Interaction between dislocations and defects plays an important role in mechanical properties. For example, self-interstitial clusters may move to decorate dislocations, thereby lowering their mobility, and dislocations can be hindered by direct intersection with clusters. We use atomic-scale computer simulation to investigate the dynamic interaction between an edge dislocation and glissile clusters with Burgers vector b = ½<111> in iron. When b is parallel to the dislocation glide plane and direct intersection does not occur, clusters can be dragged at high speed by a moving dislocation, and we present a model for drag and dislocation break-away based on the 1-D mobility of clusters. When b is inclined to the glide plane, the cluster can slip to intersect the dislocation, resulting in <100> line segments and hence restriction of slip. The implications of these results for mechanisms of irradiation effects are discussed.

11:00 AM
Cu-Precipitates Hardening in Iron Studied by Atomic-Scale Modeling: *Yuri N. Osetsky*[1]; Roger E. Stoller[2]; David J. Bacon[3]; [1]Oak Ridge National Laboratory, Computer Sci. & Math., PO Box 2008, Oak Ridge, TN 37831 USA; [2]Oak Ridge National Laboratory, Metals & Ceram., Oak Ridge, TN 37831 USA; [3]University of Liverpool, Matls. Sci. & Engrg., Brownlow Hill, Liverpool L69 3GH UK

Copper precipitates are formed in Fe-Cu ferritic alloys under irradiation and ageing and cause a significant hardening. Comprehensive discrete dislocation dynamics model to predict mechanical property changes due to microstructure evolution requires a set of rules or reactions which should be defined a priori using detailed knowledge of each dislocation-obstacle reaction. For example, in the particular case of ferritic steel with Cu precipitate hardening the Russell-Brown model is widely used. However, this model, based on simple modulus hardening and constant line tension approximations, is oversimplified. In this paper we present results of atomic-scale modeling of a moving dislocation crossing coherent Cu-precipitates of up to 5nm diameter. We demonstrate the existence of several mechanisms, such as dislocation climb, phase transformation, temperature dependence of interaction mechanism, which affect the critical resolved shear stress but cannot be resolved within the continuum approach. The implementation of atomic-scale mechanisms into continuum dislocation dynamics is discussed.

11:20 AM
Effects of Irradiation of the True Stress-Strain Constitutive Behavior of RPV Steels: *Takuya Yamamoto*[1]; G. Robert Odette[1]; [1]University of California, Dept. of Mechl. Engrg., Santa Barbara, CA 93106 USA

Effects of ˜290°C <0.05 dpa irradiation on true stress-strain s(e) properties of RPV steels were assessed. The database covers a wide range of compositions (Cu, Ni, Mn,..) and irradiation conditions (flux, fluence and temperature). The analysis separated the Luder's-type non-hardening region, with slightly higher eL after irradiation, from the strain hardening ssh(e) = s(e) - the yield stress (sy). The ssh(e) data was fit to a Kock-Mecking saturation dislocation storage and annihilation model. RPV irradiation has only a modest effect on ssh(e), with maximum decreases in the saturated ssh less than 50 MPa. The ssh(e) decreases with larger hardening (Dsy) and irradiation primarily reduces the dislocation storage term, perhaps by suppressing cross slip. In contrast to the effects of much higher dose irradiations, RPV conditions do not produce severe flow localization and reductions in tensile ductility can be predicted based on the combination of Dsy and modest decreases in ssh(e).

11:40 PM
Modeling the Constitutive Behavior of Irradiated BCC Alloys: *Athanasios Arsenlis*[1]; [1]Lawrence Livermore National Laboratory, Chmst. & Matls. Sci. Direct., PO Box 808, L-371, Livermore, CA 94550 USA

Performance degradation of bcc alloys in nuclear environments results from the formation of a high number density of nanometer scale irradiation-induced defects. An internal state variable model for the mechanical behavior of such irradiated materials has been developed. The plasticity model includes mechanisms for dislocation density growth and multiplication and for irradiation defect density evolution with dislocation interaction. The model has been modified specifically for bcc alloys by including a temperature dependent dislocation velocity law to account for the inherent lattice resistance, the

material's response to strain localization and the formation of adiabatic shear bands. The model is compared to available experimental data for Mo.

Neutron Diffraction Characterization of Mechanical Behavior: Phase Transformation

Sponsored by: ASM International: Materials Science Critical Technology Sector, Structural Materials Division, SMD-Mechanical Behavior of Materials-(Jt. ASM-MSCTS)
Program Organizers: Hahn Choo, University of Tennessee, Department of Materials Science and Engineering, Knoxville, TN 37996 USA; Camden R. Hubbard, Oak Ridge National Laboratory, Metals and Ceramics Division, Oak Ridge, TN 37831 USA; Peter K. Liaw, University of Tennessee, Materials Science and Engineering, Knoxville, TN 37996-2200 USA; Xunli Wang, Oak Ridge National Laboratory, Spallation Neutron Source, Oak Ridge, TN 37831 USA

Thursday AM Room: 3004
February 17, 2005 Location: Moscone West Convention Center

Session Chairs: Mark Daymond, Queen's University, Mechl. & Matls. Engrg., Kingston, Ontario K7L 3N6 Canada; Donald W. Brown, Los Alamos National Laboratory, Matls. Sci. & Tech. Div., Los Alamos, NM 87545 USA

8:30 AM Invited
Accelerated Aging in Uranium Niobium Alloys: *Donald W. Brown*[1]; David L. Teter[1]; Daniel J. Thoma[1]; Robert D. Field[1]; Thomas A. Sisneros[1]; Mark A.M. Bourke[1]; [1]Los Alamos National Laboratory, Matl. Sci. & Tech., MS H805, Los Alamos, NM 87544 USA

Uranium 6 weight percent niobium (U6Nb) plays an important role in our aging nuclear stockpile. Niobium is soluble in uranium at high temperature, in the body-centered cubic phase, but not at room temperature. The diffusion of niobium in uranium is rather slow, and if the alloy is quenched at moderate rates a metastable monoclinic phase is produced at room temperature. The properties that make U6Nb attractive are a strong function of the niobium content and are optimized in this metastable phase. Thus, the aging kinetics of the metastable alloy are important to the development of its mechanical behavior with time. This study was aimed at understanding the stability of the alloy through in-situ neutron diffraction measurements during accelerated aging. Samples were heated in-situ to temperatures between 100°C and 400°C and the development of the interatomic spacings monitored over roughly one-day aging times by taking diffraction patterns at 5-20 minute intervals. The observed changes in the lattice parameter are related to the decreased niobium in solution with time at temperature.

8:50 AM
In Situ Neutron Diffraction Measurement of Phase Transformation and Stress Evolution in Al/Al-Cu-Fe Composites During Vacuum Hot Pressing: *Fei Tang*[1]; Iver Eric Anderson[2]; Don W. Brown[3]; Thomas A. Sisneros[3]; Bjorn Clausen[3]; Mark A.M. Bourke[3]; [1]Oak Ridge National Laboratory, Metals & Ceram. Div., Bldg. 4515, MS6064, Oak Ridge, TN 37831 USA; [2]Ames Laboratory, Matls. & Engrg. Physics, Rm. 222, Metals Dvlp. Bldg., Ames, IA 50011 USA; [3]Los Alamos National Laboratory, LANSCE, Los Alamos, NM 87545 USA

Unlike the typical tensile residual stresses in the Al matrix of many particulate reinforced Al composites, a significant compressive residual stress was found in the Al matrix of Al/Al-Cu-Fe composites, consolidated by powder metallurgy routes. This unusual compressive stress state appeared to be related to volume expansion of the reinforcement particles that transformed from Al63Cu25Fe12 (quasicrystalline) i-phase to a less-dense (crystalline) omega-phase, during high temperature consolidation. For verification, a through-thickness neutron diffraction technique, including Rietveld analysis, was employed to monitor simultaneously the transformation and stress evolution during vacuum hot (550°C) pressing of such composites with a special compressive load frame and die set. The results revealed that the transformation onset can preceed the applied loading in the powder compact at high temperatures, but that the transformation kinetics were accelerated markedly by the applied compression. This illustrates the opportunities to validate and build materials processing models with in situ neutron diffraction. Supported by USDOE-BES.

9:10 AM
Neutron Diffraction Investigation of NiTiFe Shape-Memory Alloys During Mechanical Loading at Cryogenic Temperatures: *S. B. Shmalo*[1]; C. R. Rathod[1]; T. R. Woodruff[1]; V. Livescu[2]; B. Clausen[2]; M. A.M. Bourke[2]; W. U. Notardonato[3]; Raj Vaidyanathan[1]; [1]University of Central Florida, AMPAC/MMAE, Orlando, FL 32816 USA; [2]Los Alamos National Laboratory, Los Alamos, NM 87545 USA; [3]NASA, Kennedy Space Ctr., FL 32899 USA

NiTiFe shape-memory alloys exhibit a stress and/or temperature induced phase transformation between cubic, rhombohedral and monoclinic phases. The low hysteresis associated with the rhombohedral or R phase transformation coupled with superior fatigue properties, makes them candidates for actutator applications at low temperatures. This work reports on neutron diffraction measurements of NiTiFe shape-memory alloys during mechanical loading at cryogenic temperatures, with the objective of probing deformation in the R phase. For this purpose, a low temperature loading capability for in situ neutron diffraction measurements was implemented on the Spectrometer for Materials Research at Temperature and Stress (SMARTS) at Los Alamos National Laboratory. The in situ diffraction measurements, during loading at 216 K, observed twinning in the R phase prior to a reversible martensitic transformation to the monoclinic phase at higher stresses. Comparisons with room temperature measurements from NiTiFe were also made. This work was supported by grants from SRI, NASA (NAG3-2751) and NSF (CAREER DMR-0239512) to UCF.

9:30 AM
Lattice Strain, Phase, and Texture Evolution During Strain-Induced Martensitic Transformation at a Cryogenic Temperature: *Kaixiang Tao*[1]; James J. Wall[1]; Donald W. Brown[2]; Sven C. Vogel[2]; Mark A.M. Bourke[2]; Hahn Choo[3]; [1]University of Tennessee, Matls. Sci. & Engrg., 318 Dougherty Hall, Knoxville, TN 37996-2200 USA; [2]Los Alamos National Laboratory, MST-8, Los Alamos, NM 87545 USA; [3]Oak Ridge National Laboratory, Metals & Ceram. Div., Oak Ridge, TN 37831 USA

The strain-induced martensitic phase transformation during quasi-static uniaxial compression testing of 304L stainless steel at 300K, 268K, and 203K was investigated with in-situ time-of-flight neutron diffraction using SMARTS at Los Alamos Neutron Science Center (LANSCE). The in-situ neutron diffraction study provides bulk measurements of the evolution of phase fractions, texture, and lattice strains during the austenite to martensite transformation. To achieve a better understanding of the transformation textures and phase fraction evolution, pre-compressed samples with different strain levels were investigated with HIPPO at LANSCE, using its multidetector capabilities. The texture analysis shows that the martensite is highly textured, due to the selective phase transformation. The unique orientation relationships between the austenite and martensite result in the texture development in the parent austenite as well.

9:50 AM
Retained Austenite Stability Investigation in TRIP Steel Using Neutron Diffraction: *Jozef Zrnik*[1]; Petr Lukas[2]; Ondrej Muransky[2]; Petr Sittner[3]; Zbysek Novy[1]; [1]COMTES FHT Ltd., Pilsen 320 13 Czech Republic; [1]COMTES FHT Ltd., Pilsen 320 13 Czech Republic; [2]Institute of Nuclear Physics, Rez near Prague 250 68 Czech Republic; [3]Institute of Physics, Prague 182 21 Czech Republic

The neutron diffraction experiment was focused on transformation behavior of Si-Mn TRIP steel upon thermomechanical treatment. In order to control the TRIP effect in low alloyed TRIP steel it is necessary to understand the stability of retained austenite. The analysis was carried out with the aim to learn whether the neutron diffraction technique can successfully monitor the conditioned austenite transformation process. The relevant information on the course of transformation is extracted from neutron diffraction spectra received. The in-situ neutron diffraction experiment conducted at room temperature was focused on the quantification of retained austenite volume fraction as well as on measurement of the internal stress rising in ferrite and austenite phases during mechanical loading of specimens with different retained austenite volume fraction in complex structure. The transformation behavior of specimens with different volume fraction of retained austenite showed a similar character. The measured difference in retained austenite volume fraction seems to have no substantial effect on deformation behavior of TRIP steel.

10:10 AM Break

10:30 AM
Influence of a Deformation-Induced Phase Transformation on the Mechanical Behavior of a Co-Based Superalloy Studied by In-Situ Neutron Diffraction: *Michael Lee Benson*[1]; Tarik A. Saleh[1]; Peter K. Liaw[1]; Hahn Choo[1]; Don W. Brown[2]; Mark R. Daymond[3];

Xun-Li Wang[4]; Alexandru D. Stoica[4]; Raymond A. Buchanan[1]; Dwaine L. Klarstrom[5]; [1]University of Tennessee, Matls. Sci. & Engrg., 434 Dougherty Hall, Knoxville, TN 37996 USA; [2]Los Alamos National Laboratory, Los Alamos Neutron Sci. Ctr., Los Alamos, NM 87545 USA; [3]Queen's University, Dept. of Mechl. & Matls. Engrg., Kingston, ON K7L3N6 Canada; [4]Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA; [4]Oak Ridge National Laboratory, Spallation Neutron Source, Oak Ridge, TN 37831 USA; [5]Haynes International, Inc., Kokomo, IN 46904 USA

ULTIMET® is a cobalt-based superalloy that is metastable face centered cubic (fcc) at room temperature. The stable hexagonal close packed (hcp) phase forms via a strain-induced phase transformation. In-situ monotonic and cyclic loading experiments were performed at Los Alamos Neutron Science Center (LANSCE) and ISIS, respectively, in order to study the influence of the developing hexagonal phase on the deformation behavior of the material. During monotonic loading, the developing phase was shown to grow at the expense of grains oriented with the {220} plane normal parallel to the axial direction of the specimen. During low cycle fatigue, the new phase formed on the 12th fatigue cycle and increased in volume fraction as fatigue progressed. Also, the intensity of the hcp diffraction peak fluctuated within one fatigue cycle, suggesting some reversibility of the transformation. The study completed here should provide valuable insight into the influence of the developing phase on the mechanical behavior of the material. The author acknowledges the financial support of the National Science Foundation, the Combined Research-Curriclulm Development (CRCD) Progrmas, under EEC-9527527 and EEC-0203415, the Integrative Graduate Education and Research Training (IGERT) Program, under DGE-9987548, and the International Materials Institutes (IMI), under DMR-0231320, to the University of Tennessee, Knoxville, with Ms. M. Poats, Dr. L. Clesceri, Dr. W. Jennings, and Dr. C. Huber as contract monitors, respectively. In addition, the financial support of the Tennessee Advanced Materials Laboratory (TAML), with Prof. E. W. Plummer as director, is recognized.

10:50 AM

Influencing Parameters of Martensitic Transformation During Low Cycle Fatigue for Steel AISI 321: *Mirco Grosse*[1]; Dietmar Kalkhof[2]; Markus Niffenegger[2]; Lukas Keller[3]; [1]Paul Scherrer Institut, Spallation Neutron Source Div., Villigen 5232 Switzerland; [2]Paul Scherrer Institut, Nuclear Energy & Safety, Villigen 5232 Switzerland; [3]Paul Scherrer Institut, Lab. of Neutron Scattering, Villigen 5232 Switzerland

The present investigations include the study of the influence of thermo-mechanical manufacturing conditions and of low cycle fatigue parameters, (load amplitude, load frequency, cycle number and fatigue test temperature) on content and texture of the martensite. The material investigated was the austenitic stainless steel AISI 321. This steel is commonly used as material for pipes of cooling circuits in nuclear power plant. The content of martensite after the LCF test and the martensite texture were determined by neutron diffraction using the DMC diffractometer at SINQ/PSI (Switzerland). Whereas no influence was found for the load frequency the martensite content linear increases with increasing cycle number and load amplitude. It decreases exponentially with increasing LCF test temperature. The thermo-mechanical manufacturing conditions show a strong influence. The amount of martensite formed during LCF is much higher after cold rolling than after solution annealing as final manufacturing process.

11:10 AM

On-Line Low Cycle Stress Rig Neutron Diffraction Study of a Martensite Phase Transformation in Stainless Steel AISI 321 Ad Interim High Cycle Fatigued: Yu. V. Taran[1]; *M. R. Daymond*[2]; E. C. Oliver[2]; J. Schreiber[3]; [1]Joint Institute for Nuclear Research, Frank Lab. of Neutron Physics, Dubna, Moscow Region 141980 Russia; [2]Rutherford Appleton Laboratory, ISIS, Chilton, Didcot, Oxon OX11 0QX UK; [3]Fraunhofer Institute for Nondestructive Testing, EADQ, Dresden D-01326 Germany

Earlier we have described results of the tensile test of samples from a steel AISI 321 ad interim cycle fatigued at frequency of 5 Hz (HCF-samples) and 0.5 Hz (LCF-samples). In HCF-samples the elastic constants of austenite and martensite were found out to be strongly different as against LCF-samples in which they are close. More over, the ratio of axial and transverse elastic constants for martensite in the HCF-samples is almost twice that observed 0.28-0.30 in austenite and in both phases of the LCF-samples. The mechanism for this unusual behaviour is unclear, but may be linked to the shape of the martensite. One of HCF-samples was anew tested using the in situ stress rig in : 1) low cycle mode at a frequency of 0.1 Hz to increase the fatigue level, and 2) a quasistatic mode to measure the applied stress-elastic strain responses of both phases. The HCF-LCF-transformation was studied at increasing martensite fraction from 5 to 19 Wt. %. It is exerted a week influence on mechanical properties of the sample.

11:30 AM

Spatially Resolved Neutron Diffraction Measurement of Heterogeneous Stress-Induced Phase Transformation in a Superelastic NiTi Disc: *C. R. Rathod*[1]; S. B. Shmalo[1]; B. Clausen[2]; M. A.M. Bourke[2]; Raj Vaidyanathan[1]; [1]University of Central Florida, AMPAC/MMAE, Orlando, FL 32816 USA; [2]Los Alamos National Laboratory, Los Alamos, NM 87545 USA

Previous work has reported on the use of neutron diffraction to probe predominantly homogeneous stress-induced transformations in NiTi associated with uniaxial stress states (Vaidyanathan et al, Acta Mater 1999). In the following, we report on neutron diffraction measurements from a NiTi disk specimen loaded laterally in compression and associated with a macroscopically heterogeneous stress state. Measurements were performed on the Spectrometer for Materials Research at Temperature and Stress (SMARTS) at Los Alamos National Laboratory in a spatially resolved mode. Neutron spectra confirm the presence of both monoclinic and cubic phases of NiTi, with the respective volume fractions depending on the location of the measurements (and the corresponding stress state). The neutron diffraction measurements of the strain, texture and phase volume fraction offer insight into accommodation mechanisms as the cubic and monoclinic phases co-exist in a macroscopically heterogeneous stress state. This work was supported by a grant from NSF (CAREER DMR-0239512) to UCF.

Powder Metallurgy Research and Development in the Transportation Industry: Nano-Materials, Intermetallics, Amorphous and Composites - P/M Developments

Sponsored by: Materials Processing and Manufacturing Division, MPMD-Powder Materials Committee

Program Organizer: James W. Sears, South Dakota School of Mines & Technology, Additive Manufacturing Laboratory, Rapid City, SD 57701 USA

Thursday AM
February 17, 2005

Room: 3008
Location: Moscone West Convention Center

Session Chair: James W. Sears, South Dakota School of Mines & Technology, Additive Mfg. Lab., Rapid City, SD 57701 USA

8:30 AM

Preliminary Evaluation of Equal Channel Angular Extrusion Followed by Combustion Synthesis of TiAl: *K. Morsi*[1]; Sandeep Goyal[1]; [1]San Diego State University, Mechl. Engrg., 5500 Campanile Dr., San Diego, CA 92182 USA

Titanium aluminides are one of the most promising intermetallics today. They have previously been processed using a variety of routes to generate different microstructures. Recently, severe plastic deformation by equal channel angular extrusion (ECAE) has been found to be a viable method for producing ultrafine materials in bulk form. The work presented in this paper involves preliminary investigations of ECAE of elemental titanium and aluminum powders (one pass) followed by combustion synthesis. The effect of processing (ECAE vs. uniaxial pressing) on the reaction characteristics, product homogeneity and microstructure is presented.

8:55 AM

Plasma Synthesis of Ultrafine AlTi-TiC Composites: *Lirong Tong*[1]; Ramana G. Reddy[1]; [1]University of Alabama, Dept. of Metallurgl. & Matls. Engrg., PO Box 870202, Tuscaloosa, AL 35401 USA

A novel in_situ processing technique of ultrafine AlTi-TiC composite by thermal plasma was developed to investigate synthesis of ultrafine AlTi-TiC composite powders. A basic understanding of thermodynamics of synthesis of ultrafine AlTi-TiC composite powders is essential. Thermodynamic analysis was performed to predict conditions of synthesis and recovery rate of ultrafine AlTi-TiC composite powders. The paper emphasizes on the investigation of feeding rate, input power, mole ratio and other process parameters of synthesis of ultrafine AlTi-TiC composite powders by thermal plasma. The experimental results showed that ultrafine AlTi-TiC composite powders can be synthesized and the average size of ultrafine AlTi-TiC composite powders was less than 200 nm.

9:20 AM
Powder Extrusion of Nanostructured Aluminum Alloy Created by Machining: *Balkrishna C. Rao*[1]; Srinivasan Chandrasekar[1]; Kevin P. Trumble[1]; W. Dale Compton[1]; [1]Purdue University, Ctr. for Matls. Procg. & Tribology, Coll. of Engrg., 315 N. Grant St., W. Lafayette, IN 47907-2023 USA

An exploratory study has been made of extrusion of nanostructured Aluminum 6061-T6 particulate derived from machining chips. For this purpose, chips with nanocrystalline microstructure were created by machining bulk Al6061-T6 alloy. The hardness of the chips was found to be greater than that of the same alloy produced by Equal Channel Deformation Processing. The chips were converted into particulate with an average particle size of ~75 micrometers by attrition milling. Monolithic bulk forms of the 6061-T6 were created by axisymmetric cold extrusion of the particulate through a conical die. Additionally, bulk composites were produced by cold extrusion of mixtures of the 6061-T6 particulate and commercially pure aluminum particulate. Microstructure, mechanical and physical properties of the extruded bulk forms are characterized and compared with those of conventionally processed Al6061-T6 alloy. Some of the attractive advantages of the ultrafine-grained Al6061-T6 extruded samples are highlighted with reference to the results. Implications to up-cycling of machining chips produced in discrete product machining operations are also discussed.

9:45 AM
Compressive Behavior of a Novel Aluminum Metal Matrix Composite: *Jichun Ye*[1]; Bing Q. Han[1]; Julie M. Schoenung[1]; [1]University of California, Dept. of Cheml. Engrg. & Matls. Sci., 3118 Bainer Hall, One Shields Ave., Davis, CA 95616 USA

Al 5083 and B4C were cryomilled in liquid nitrogen to form a composite of B4C particles in nanocrystalline Al. The cryomilled composite powders were blended with coarse-grained Al 5083. The blended powders were consolidated using cold isostatic pressing and extrusion. The resultant composite is a complicated materials system with three phases, 10 wt. % B4C, 50 wt. % coarse-grained Al 5083 and the balance nanocrystalline Al 5083. B4C and nanocrystalline Al contribute to the high strength, while coarse-grained Al was introduced to achieve ductility because of the dislocation activity it provides. Compression tests were conducted on this composite at various temperatures to examine its mechanical behavior. The results show that this composite exhibits an extremely high yield strength of 1150 MPa at room temperature with 2.5% elongation. The microstructure of this tri-modal composite was investigated, and the relationship between the excellent mechanical behavior and the microstructure are discussed.

10:10 AM
Effects of Non-Equilibrium Phases on Mechanical Properties of Al Composites Processed by Mechanical Alloying: *Kwang Seon Shin*[1]; *Woo Kil Jang*[1]; [1]Seoul National University, Sch. of Matls. Sci. & Engrg., San 56-1 Shinrim-dong Kwanak-gu, Seoul 151-742 Korea

The effects of non-equilibrium phases on the microstructures and mechanical properties of Al composites were investigated in the present study. The non-equilibrium phases such as quasicrystalline phase and amorphous powders were utilized as strengtheners in this study. Powders of the quasicrystalline phase were produced by casting and subsequent milling. The amorphous powders were produced by the gas atomization method. Mechanical alloying process was utilized in order to produce appropriate powders for the Al matrix composites reinforced with either quasicrystalline or amorphous phases. The composite powders were canned in the Al can and extruded at elevated temperatures. The microstructures of the extrusions were examined by OM and SEM. In order to investigate the mechanical properties of the extrusions, hardness and compression tests were carried out. It was found that the mechanical properties and thermal stability of the Al composites reinforced with quasicrystalline phase or bulk amorphous phase significantly increased compared with those of the conventional Al matrix composites.

10:35 AM
High Cycle Fatigue Studies on Devitrified Amorphous Aluminum Alloys: S. Qi[1]; *P. Wesseling*[1]; J. J. Lewandowski[1]; [1]Case Western Reserve University, Dept. of Matls. Sci. & Engrg., 10900 Euclid Ave., Cleveland, OH 44106-7204 USA

Devitrified amorphous aluminum rods produced by extrusion of amorphous aluminum powders were used in this investigation. Deformation processing of the amorphous aluminum alloy produced a nanocomposite structure possessing very high bend strength and non-zero ductility with ductile fracture as the fracture mode. Smooth bend bar specimens were prepared from these rods to conduct high cycle fatigue tests over a wide range of stresses and test temperatures. The high cycle fatigue behavior will be compared to the behavior of other aluminum alloys.

Rare Earths: Science, Technology and Applications V: Rare Earths

Sponsored by: Light Metals Division, LMD-Reactive Metals Committee
Program Organizers: Renato G. Bautista, University of Nevada, Department of Chemical and Metallurgical Engineering, Reno, NV 89557-0136 USA; Dhanesh Chandra, University of Nevada, Chemical and Metallurgical Engineering, Reno, NV 89557 USA; John N. Hryn, Argonne National Laboratory, Argonne, IL 60439-4815 USA

Thursday AM — Room: 3001
February 17, 2005 — Location: Moscone West Convention Center

Session Chairs: Scott W. Jorgensen, General Motors Corporation, Cheml. & Environml. Scis. Lab., Warren, MI 48090-9055 USA; Dhanesh Chandra, University of Nevada, Cheml. & Metallurgl. Engrg., Reno, NV 89557 USA

8:30 AM Keynote
The Influence of Rare Earths on the Corrosion Resistance of High Temperature Materials: *David A. Shifler*[1]; [1]Naval Surface Warfare Center, Marine Corrosion Branch, 9500 MacArthur Blvd., W. Bethesda, MD 20817-5700 USA

Selected reactive elements such as zirconium, hafnium, yttrium, and rare earths or the presence of selected oxide dispersions added to selected alloys or coatings often have shown marked improvement of the oxidation resistance, corrosion resistance, and scale adhesion. These effects may include (1) more rapid formation of a continuous oxide scale, (2) reduction in the oxidation rate, (3) improved scale adherence, (4) a change in the scale-forming reaction location from the scale-gas interface to scale-alloy interface. Reactive elements improve the oxidation resistance and high-temperature corrosion of many high temperature alloys, particularly if the resistance is dependent on oxide formation. This paper will provide an overview of the bases by which rare earths and other reactive elements influence the oxidation and high temperature corrosion resistance of materials.

8:50 AM Invited
Production of Value Added Rare Earths from Monazite by Solvent Extraction: *L. N. Maharana*[1]; V. R. Nair[1]; [1]Indian Rare Earths Limited, Rare Earths Div., Udyogamandal-683 501, Kerala State India

The Rare Earths Division of Indian Rare Earths Limited (IREL) started processing of monazite in 1952. IREL is one of the pioneers in the processing of. monazite. Over the years IREL perfected the monazite processing technology and is producing rare earth compounds, trisodium phosphate, thorium and uranium chemicals at present. In recent times IREL has focussed its attention to produce value added high purity rare earth chemicals to meet the demand for these materials in the international and indigenous markets. The R&D laboratory of IREL has developed several processes for the separation of rare earths based on solvent extraction technology. These solvent extraction processes developed were scaled up and implemented on plant scale. The solvent extraction separation processes employed at IREL include separation of cerium, neodymium and samarium by using PC-88A(mono-2-ethyl hexyl ester of mono-2-ethyl hexyl phosphonic acid) and the separation of yttrium using the quarternary ammonium compound Aliquat-336(tri octyl methyl ammonium chloride) as the extractants. The details of the solvent extraction process development and flow sheets employed by IREL will be presented in this paper.

9:10 AM
Novel Functional and High Temperature Applications of Nanocrystalline Rare Earth Phosphate Coatings and Composites: *K. G.K. Warrier*[1]; K. Rajesh[1]; R. Rohith[1]; V. R. Nair[2]; [1]Regional Research Laboratory (Council of Scientific & Industrial Research), Ceram. Tech. Div., Thiruvananthapuram 695 019 India; [2]Indian Rare Earths Limited, Udyogamandal India

The range of rare earth phosphates has been identified for their high temperature phase stability and high melting points. Non reactivity with certain other ceramic materials such as alumina, use of the rare earth phosphate as an interface in alumina matrix composites,

machinability of the alumina-rare earth composites, possible applications as catalysts and the luminescent and optical properties have been subject of investigation over the last decade. Synthesis and characterization of nano crystalline rare earth phosphate has been of recent interest in view of the wide possibilities of this range of materials for various applications. The present work relates to the synthesis of 30-50 nm size particles of lanthanum and cerium phosphates by sol-gel colloidal technique starting from respective nitrates. The gel to phosphate transformation, the high temperature stability, densification characteristics at as low temperatures as 1400°C are presented. The electrical properties of these phosphates indicate low dielectric constant and loss factors. Nano crystalline sintered rare earth phosphate also indicates high temperature deformation behaviour. Lanthanum phosphate coatings on various substrates have been developed and certain features of such coatings have also been investigated. The paper covers an overview of the range novel characteristics of the rare earth phosphates. Experimental details of synthesis in nano crystalline phosphate and certain novel findings are presented. The possibility of practical applications of this range of materials for a variety of applications is highlighted.

9:30 AM

Ductile Intermetallic Compounds! The Rare Earth RM B2 CsCl-Type Intermetallics: *Karl A. Gschneidner*[1]; Alan M. Russell[1]; Alexandra O. Pecharsky[1]; Zhehua Zhang[1]; James R. Morris[1]; Tom A. Lograsso[1]; C. H. Chester Lo[1]; Yiying Ye[1]; [1]Iowa State University, Ames Lab., Ames, IA 50011-3020 USA

A number of the rare earth intermetallic B2 CsCl family of compounds (~100 members) exhibit unprecedented large ductilities at room temperature, up to ~25% elongation at failure. These compounds are fully ordered, stoichiometric, and in general line compounds. To date quantitative measurements have been made on RCu (R = Y, Dy and Er), YAg and (Tb<0.88>Dy<0.12>)Zn. Of the five compounds only the RZn phase is brittle. YAg is the most ductile compound examined to date with an elongation of 27% at failure with a maximum tensile strength of ~150 MPa (comparable to a typical solid solution aluminum alloy). Preliminary measurements indicate ten other RM phases are also ductile RCu (R = Gd, Ho, Dy), RAg (R = Ce, Nd and Er), YRh, YIn, ErIr and ErAu. The results of mechanical property tests and ab initio calculations, including band structures and unstable stacking fault energies, will be discussed.

9:50 AM

Microstructural Investigation of Mixed Rare Earth Iron Borides Processed Via Melt Spinning and Gas Atomization: *Nick Buelow*[1]; Iver E. Anderson[2]; William McCallum[2]; Matthew Kramer[2]; Wei Tang[2]; Kevin W. Dennis[2]; [1]Iowa State University, Matls. Sci. & Engrg., 221 Metals Dvlp., Ames, IA 50014 USA; [2]Ames Laboratory, Matls. & Engrg. Physics, Ames, IA USA

Novel mixed rare earth iron boride (MRE-Fe-B) permanent magnet (PM) alloy combines Nd, Y, and Dy with Fe, B, and other substitutions to help stabilize the temperature dependent magnetic properties remenance, coercivity, and BH_{max}. MRE-Fe-B has demonstrated stabilization of the temperature dependent magnetic properties beyond 200°C; whereas, $Nd_2Fe_{14}B$ based PMs have magnetic properties that deteriorate rapidly at ~125°C. The challenge has been to adjust alloy designs and annealing treatments to convert the developments made with melt spun ribbons into gas atomized powders with fine spherical particulate form, preferred for polymer bonding. Synthesis of an optimum fine uniform microstructure for the $MRE_2Fe_{14}B$ alloys is being accomplished through melt spinning and high pressure gas atomization. Both processes can boast cooling rates of ~10^{6o}C/s which promote the formation of similar amorphous and nanoscaled structures, but with differences in the nucleated phases and growth orientations. Support from USDOE-EE is acknowledged through contract no. W-7405-Eng-82.

10:10 AM Break

10:20 AM

Crystal Growth of RE-Si-Ge Magnetocaloric Compounds: *Deborah L. Schlagel*[1]; Thomas A. Lograsso[1]; Alexandra O. Pecharsky[1]; Juraci A. Sampaio[1]; [1]Ames Laboratory, Matls. & Engrg. Physics Prog., Ames, IA 50011 USA

Single crystals of RE5(SixGe1-x)4 have been prepared by both the Bridgman and by the tri-arc crystal pulling method. Bridgman grown crystals, grown in welded tungsten crucibles, contained large grains but were severely cracked due to alloy/crucible thermal mismatch. The Tri-arc method had the advantage of being crucible-less and the usable crystal size has been increased with this method. Overall, the bulk crystal solidified in the monoclinic phase with a slight increase in Si content and decrease in Ge content as the growth proceeded. This increase in Si:Ge ratio resulted in a slight increase in lattice parameter of the monoclinic phase and an increase in the magnetostructural transformation temperature of ΔT = 10K. AC susceptibility and differential scanning calorimetry (DSC) measurements indicated a small fraction of orthorhombic phase was present throughout the ingot which accounts for the decrease in MCE values along the length of the ingot.

10:40 AM

Amorphization and Nanocrystallization of the Intermetallic Compound $TbFe_2$ by Ball Milling: *Jiahong Zhu*[1]; Zigui Lu[1]; Chain T. Liu[2]; Joe A. Horton[3]; [1]Tennessee Technological University, Dept. of Mechl. Engrg., 115 W. 10th St., Box 5014, Cookeville, TN 38505 USA; [2]Oak Ridge National Laboratory, Metals & Ceram. Div., PO Box 2008, MS 6115, Oak Ridge, TN 37831 USA; [3]Oak Ridge National Laboratory, Metals & Ceram. Div., PO Box 2008, MS 6115, Oak Ridge, TN 37831 USA

The rare earth-transition metal system based on $TbFe_2$ possesses huge magnetostriction. However, due to its large magnetocrystalline anisotropy, a high magnetic filed is required to obtain the desired magnetostrictive strains. One way to reduce the magnetostrictive anisotropy and thus the actuation field is to refine the grains to the nanometer scale. In this paper, we tried to produce the nano-sized grain structures in binary $TbFe_2$ via amorphization by high-energy ball milling followed by nanocrsytallization treatment. To separate the different stages of ball milling process, the formation of an amorphous phase starting from an intermetallic compound was investigated. Experimental conditions were described under which the intermetallic compound $TbFe_2$ became amorphous. The crystallization behavior of the amorphous phase was studied using a DSC apparatus. The optimal conditions to generate nanocrystalline materials were determined. The magnetostrictive properties of amorphous and nanocrystallized $TbFe_2$ were evaluated by the standard strain gauge method.

11:00 AM

Characterization of R5(SixGe1-x)4 Alloys, Where R is Gd, Tb, Dy and Er: *Ozan Ugurlu*[1]; Scott L. Chumbley[1]; Deborah L. Schlagel[2]; Thomas A. Lograsso[4]; Alexandra O. Pecharsky[3]; [1]Iowa State University/Ames Laboratory, Matls. Sci. & Engrg., 206 Wilhelm Hall, Ames, IA 50011 USA; [2]Ames Laboratory, 110 Metals Dvlp., Ames, IA 50011 USA; [3]Ames Laboratory, 239 Spedding Hall, Ames, IA 50011 USA; [4]Ames Laboratory, Matls. Sci. & Engrg., 111 Metals Dvlp., Ames, IA 50011 USA

Bulk microstructures of R5(SixGe1-x)4 alloys, where R is Gd, Tb, Dy and Er, have been examined using transmission (TEM) and scanning (SEM) electron microscopy. The microstructure of all alloys consisted of large grains with linear features present within the grains. The features in general are on the order of 1 micron or less in width and hundreds of microns in length, and are seen in all alloys independent of their crystal structure. Single crystals of Gd5Si2Ge2 have been used to study the crystal orientation of the linear features by using a combination of back-reflection Laue x-ray diffraction and SEM. Systematic tilting experiments of a single crystal of Gd5Si2Ge2 with controlled polishing angles showed that these linear features grow in specific directions as thin plates. Energy Dispersive Spectrometry (EDS) results revealed that the plates have a composition approximating R5(SixGe1-x)3 type phases in all the alloys systems studied, and TEM studies using electron diffraction and high resolution TEM confirmed this. These results verify an earlier study that suggested the features might possibly be a Widmanstatten structure that forms during sample preparation.

11:20 AM

Structure/Properties Relationships in the Pr2Ni1.5-xSi2.5+x Alloys Series, Where $0 \le x \le 1$: *Alexandra O. Pecharsky*[1]; Karl A. Gschneidner[1]; Kevin W. Dennis[1]; R. William McCallum[1]; [1]Iowa State University, Ames Lab., Ames, IA 50011-3020 USA

The $Pr_2Ni_{1.5-x}Si_{2.5+x}$ alloys, where $0 \le x \le 1$, adopt the AlB2 structure type with the P6/mmm space group symmetry. These alloys exist over an extended solid solution at 33.3 at.% of Pr and a random occupation of the boron sites by Ni and Si. This crystal structure belongs to one of the simplest and most extended classes of structure types which consists of a trigonal prismatic arrangement of the large atoms. The trigonal prisms form the columns with the Pr atoms in the corners and the Ni/Si atoms located in the center of each trigonal prism. The axes of the trigonal prisms are collinear and their bases are coplanar. The specific heat and magnetic measurements of the as-prepared alloys indicate antiferromagnetic ordering at low temperatures (~5K), which depends upon the Ni/Si ratio. The samples appear to undergo a metamagnetic transition at ~10 kOe, where the critical field also depends upon the Ni/Si ratio.

11:40 AM Invited
Structure and Magnetocaloric Properties of Fe-Doped HoTiGe Compound: *Ben Baumgold*[1]; V. Provenzano[1]; A. J. Shapiro[1]; R. D. Shull[1]; [1]National Institute of Standards and Technology, Magnetic Matls. Grp., 100 Bureau Dr., MS-8552, Gaithersburg, MD 20899 USA

The structure and the magnetocaloric properties of the iron-doped HoTiGe compound have been studied by means of SEM, EDS, XRD, and SQUID magnetometry. Consistent with earlier studies by Tegus and his co-workers on the iron-free compound (1-3), the iron-containing compound exhibited a highly textured microstructure and a antiferromagnetic-to-paramagnetic phase transition near 90 K with the attendant magnetocaloric effect peak centered at the same temperature. However, the iron-doped alloy contained three additional minor phases not present in the HoTiGe compound, two of which were titanium and iron-rich, while the third phase was Ho-rich. The corresponding magnetization versus temperature data clearly showed the presence of two additional magnetic phase transitions, occurring at about 2 K and at 10 K. Correspondingly, the magnetic entropy change, -DS, versus temperature plots, computed from the isothermal magnetization data, showed the presence of magnetocaloric effect peaks, also centered at about 2 K and 10 K, whose respective magnitudes are factors of 6 and 2 larger than that for the 90 K peak. It is believed that the minor phases present in the iron-doped alloy give rise both to the two additional low temperature magnetic phase transitions and to the coincident DS peaks. These results have positive implications for cryogenic magnetic refrigeration applications, including detector cooling in space-based systems and hydrogen liquefaction, which will be important for a future hydrogen-based economy.

Recycling - General Sessions: Post-Consumer Recycling

Sponsored by: Extraction & Processing Division, Light Metals Division, LMD/EPD-Recycling Committee
Program Organizer: Mark E. Schlesinger, University of Missouri, Department of Metallurgical Engineering, Rolla, MO 65409-0001 USA

Thursday AM Room: 2011
February 17, 2005 Location: Moscone West Convention Center

Session Chair: Michael L. Free, University of Utah, Dept. of Metall. Engrg., Salt Lake City, UT 84112 USA; Markus A. Reuter, Delft University of Technology, Delft 2628 The Netherlands

8:30 AM
Differential Recycling Fees for Containers Made of Multiple Materials: *Esher Hsu*[1]; Chen-Ming Kuo[2]; [1]National Taipei University, Dept. of Stats., 67 Sect. 3, Min-Sheng E. Rd., Taipei 104 Taiwan; [2]I-Shou University, Dept. of Mechl. Engrg., 1 Sect. 1, Hsueh-Cheng Rd., Ta-Hsu, Kaohsiung 84008 Taiwan

In Taiwan, manufacturers and importers have responsibility to pay the recycling fees for the packaging containers based upon the recycling rates and the amount produced or imported. The containers made of multiple materials may cause more impact on environment and recycling cost than these of simple materials. This paper aims to explore the feasibility of differential rates for containers with multiple materials. A sampling survey is employed to estimate environmental impact, reused value, and recycling cost, which are further used to calculate the differential recycling rates; whereas the economic impact is also explored to evaluate its feasibility. Study results show that charging extra fee for the containers with multiple materials based upon the additional recycling cost of complicate materials is a good way to lead producers to develop more environmentally friendly products with simple material, but this could also cause economic impact more or less.

8:55 AM
The Calculation of the Recycling Rate of Cars: *Markus Andreas Reuter*[1]; Antoinette van Schaik[1]; [1]TU Delft, Applied Earth Scis., Mijnbouwstraat 120, Delft 2628 RX The Netherlands

This paper will provide an overview of the present methods used for the calculation of recycling rates also that provided by the ISO norm. An alternative improved method will be discussed and presented based on the inclusion of statistical distribution functions. The method will be illustrated by detailed calculations to illustrate the difference between present superficial and non-rigorous methods and the method discussed in this paper. It will also suggest that the whole chain of recycling has to be controlled in order to arrive at suitable recycling rate numbers which have enough basis to satisfy car industry during the type approval of vehicles for example but also to provide the insight and numbers required by the recycling industry to evaluate their own processes.

9:20 AM
Identifying Economic and Scrap Reuse Benefits of Light Metals Sorting Technologies: Preston P. Li[1]; Sigrid Guldberg[2]; Hans Ole Riddervold[2]; *Randolph E. Kirchain*[1]; [1]Massachusetts Institute of Technology, Matls. Sys. Lab., Rm. E40-421, 77 Mass. Ave., Cambridge, MA 02139 USA; [2]Hydro Aluminum, Drammensveien 264, N-0240, Oslo Norway

The changing pattern of aluminum scrap usage has created material reuse challenges for the industry. For instance, mixed scraps consisting of wrought and cast alloys often cannot be directly re-melted and reused due to compositional incompatibility. Various new sorting technologies promise to address these challenges. It is critical to understand how, when, and to what extent sorting should be applied in different circumstances. This paper examines the use of linear programming methods to identify economically efficient sorting strategies and their impact on scrap usage. Economic efficiency was tested for various states of scrap material supply, finished good demand, sorting technology type, and sorting performance. The model can be used to identify optimized specific sorting schemes. The overall goal is to support industry decision-making regarding the application of sorting technologies to increase scrap use and lower production costs.

9:45 AM
A Comparison of the Modelling of Comminution and Liberation in Minerals Processing and Shredding of Passenger Vehicles: *Antoinette van Schaik*[1]; Markus Andreas Reuter[1]; [1]Delft University of Technology, Mijnbouwstraat 120, Delft 2628 RX The Netherlands

The material connections and combinations in car design determine the particle size reduction and the degree of liberation during shredding, which affects the composition of the intermediate recycling streams and the efficiency of physical separation. The quality of intermediate recycling products is important for optimizing material recovery in metallurgical processing, to achieve the high recycling rates required by the European Union. Modelling of liberation is extensively applied in classical minerals processing. However, modelling of liberation for consumer goods differs fundamentally from minerals processing. This paper investigates the fundamental differences between comminution and liberation in minerals processing and shredding modern consumer goods, such as the car. From this research, it will become clear to what extent classical minerals processing approaches can be used to model the design and shredding of the car. A clear direction will be given for future modelling and optimisation work on the recycling of end-of-life vehicles.

10:10 AM Break

10:40 AM
Removal and Recovery of Solder from Printed Circuit Boards: Robert W. Gibson[1]; *Derek J. Fray*[1]; [1]University of Cambridge, Dept. of Matls. Sci. & Metall., Pembroke St., Cambridge CB2 3QZ UK

The quantity of electronic scrap is growing almost exponentially, and this needs to be recycled into the constituent metals and components rather than landfilled. This paper will concentrate on the removal of solder from both complete printed circuit boards and shredded boards. The leachant used was fluoroboric acid with Ti(IV) added as an oxidant. It was found that the solder was dissolved in the leachant and could be subsequently recoved by electrowinning. For complete printed circuit boards, the electronic components either fell off the boards or could be eaily removed, and were found to have been completely unaffected by the leachant.

11:10 AM
Feasibility Study on the Recycling of Cadmium-Telluride Photovoltaic Modules: *Wenming Wang*[1]; *Vasilis M. Fthenakis*[1]; [1]Brookhaven National Laboratory, Environml. Scis. Dept., Bldg. 830, Upton, NY 11973 USA

Cadmium and selenium are used to manufacture thin film photovoltaic modules. The environmental concerns associated with these heavy metals have prompted recycling of the PV modules. A hydrometallurgical processing route has been investigated at the Brookhaven National Laboratory. Cadmium and tellurium were stripped from PV module substrates by leaching with hydrogen and dilute sulfuric acid in a tumbling machine. Both were readily solubilized with low strength acid (1.0M H2SO4) at ambient temperature. Leaching the PV module scraps completely extracted both cadmium and tellurium. In the separation

step, cation exchange resin completely separated cadmium from tellurium-rich leach liquor of 0.5 M H2SO4. Ion exchange column studies showed that elution of the resin with high strength H2SO4 generated concentrated cadmium solution, from which cadmium was recovered by electrowinning.

11:35 AM
Recovery of Metals from Dilute Solutions by Pulsed Electrodeposition: *Michael L. Free*[1]; [1]University of Utah, Metallurgl. Engrg., 135 S. 1460 E., Rm. 412, Salt Lake City, UT 84112 USA

Many industrial solutions contain low levels of dissolved metals that can be recovered and recycled into useful products. This study shows the effects of various process parameters on the recovery of metals from dilute solutions using pulsed electrodeposition.

Superalloys and Coatings for High Temperature Applications: Superalloys - III

Sponsored by: Structural Materials Division, SMD-High Temperature Alloys Committee, SMD-Corrosion and Environmental Effects Committee-(Jt. ASM-MSCTS), High Temperature Materials Committee of IoM3

Program Organizers: Roger C. Reed, University of British Columbia, Department of Metals and Materials Engineering, Vancouver, British Columbia V6T 1Z4 Canada; Richard S. Bellows, Solar Turbines, Inc., Materials and Process Engineering, San Diego, CA 92186-5376 USA; Qiang (Charles) Feng, University of Michigan, Department of Materials Science and Engineering, Ann Arbor, MI 48109 USA; Tim Gabb, NASA Glenn Research Center, Cleveland, OH 44135 USA; John Nicholls, Cranfield University, Bedfordshire MK43 OAL UK; Bruce A. Pint, Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA

Thursday AM — Room: Nob Hill A/B
February 17, 2005 — Location: San Francisco Marriott

Session Chairs: Roger C. Reed, University of British Columbia, Vancouver, BC V6T 1Z4 Canada; Qiang (Charles) Feng, University of Michigan, Dept. of Matls. Sci. & Engrg., Ann Arbor, MI 48109 USA

8:30 AM
Comparison of Low Coefficient of Thermal Expansion (CTE) Nickel Alloys Containing 12.5% Chromium: *David E. Alman*[1]; Paul D. Jablonski[1]; [1]U.S. Department of Energy, Albany Rsch. Ctr., 1450 Queen Ave., SW, Albany, OR 97321 USA

Research aimed at formulating low CTE nickel-base superalloys for intermediate-temperature solid oxide fuel cells (SOFCs) is reported. Alloys based on the composition Ni-12.5wt % Cr were modified with either W or Mo to lower CTE to on the order of 12.5 x 10-6 C-1. Mn was added to impart the formation of an outer Cr-Mn spinel and thus minimize chromium vaporization in moist environments. Linear variable differential transducer (LVDT) based dilatometer measurements were used to determine the thermal expansion of the alloys in accordance with ASTM standard E-228-85. Characterisation was performed by XRD and EDS and the results compared to thermodynamic predictions. Oxidation tests (in dry and wet air) were conducted at 750 and 800°C. The results were compared to the behavior of a commercial Fe-22Cr (Crofer 22APU) and Ni-22Cr (Haynes 230) alloys. The oxidation resistance of the low CTE-alloys was intermediate between Crofer 22APU and Haynes 230.

8:55 AM
High-Cycle Corrosion-Fatigue Investigation of the Nickel-Based Alloy, Haynes 2000: *Rejanah V. Steward*[1]; Ray A. Buchanan[1]; Peter K. Liaw[1]; Douglas E. Fielden[1]; Dwaine L. Klarstrom[2]; [1]University of Tennessee, Matls. Sci. & Engrg., 434 Dougherty Hall, Knoxville, TN 37996-2200 USA; [2]Haynes International, Inc., 1020 W. Park Ave., Kokomo, IN 46904-9013 USA

Generally, deterioration of fatigue properties is caused by preferential corrosion of the distorted metal due to rapid dissolution of atoms exposed by slip band formation, which creates a high stress concentration and subsequent crack initiation. Metals that are susceptible to corrosion are intuitively expected to be susceptible to corrosion fatigue. In this investigation, the corrosion behavior of Haynes C2000, Ni-23Cr-16Mo-1.6Cu weight % (wt. %), immersed in aerated and deaerated 3.5 wt.% sodium chloride solutions, potentially detrimental metal-chloride solutions, and simulated mechanically-perturbed environments have been studied to substantiate corrosion-fatigue failure suppositions. High-cycle fatigue tests were conducted in air at a frequency of 20 Hz. X-ray photoelectron spectroscopy characterizes the alloy as having a predominantly Cr2O3 protective film, and the repassivation kinetics appears to be immediate upon film breakage. The fracture morphology is that of a faceted cleavage nature. The corrosion fatigue results are expected to be lower than those observed in air.

9:15 AM
Effect of Carbon Additions on the Mechanical Properties of a Single Crystal Ni-Base Superalloy: *Elyssa Renee Cutler*[1]; Khalid A. Al-Jarba[1]; Gerhard E. Fuchs[1]; [1]University of Florida, Matls. Sci. & Engrg., PO Box 116400, Gainesville, FL 32611 USA

Carbon was added to a model single crystal Ni-base alloy, LMSX-1, to reduce casting defects. Mechanical testing including creep, tensile and fatigue tests were carried out. Fractography revealed distinct changes in behavior according to carbon level. Samples were tested in both a heat treated and overaged condition. Though the increases in carbon content improved castability, creep lives were drastically reduced. No steady state creep rates or incubation times were seen in any samples. Carbide compositions and morphologies were altered by exposure during creep testing. Microstructural changes caused by increasing carbon additions were detrimental to mechanical properties. A preliminary Larsen-Miller curve was developed.

9:35 AM
Electrical Monitoring of Microstructural Fluctuations in Waspaloy as a Function of Thermal Exposure: *Siva Kumar*[1]; Rosario A. Gerhardt[1]; [1]Georgia Institute of Technology, Sch. of Matls. Sci. & Engrg., 771 Ferst Dr., Atlanta, GA 30332-0245 USA

Microstructural evolution in Waspaloy, an age-hardenable nickel-base superalloy, was investigated as a function of thermal exposure to 1400ºF for times up to 2502 hours. Specimens sampled at several intermediate exposure times were characterized using impedance spectroscopy, optical microscopy, SEM, XRD and stereology. Repetitive upward and downward trends were noted in the lattice parameter and the composition in all cases. Similar fluctuations were apparent in the volume fraction (Vv) of the primary g¢ precipitates with progressive thermal exposure. An inverse correlation between Vv and Y-max, an electrically derived parameter was obtained. Since the average g grain size also varied considerably during the length of the experiment, solutionizing and aging experiments are ongoing in order to determine if the fluctuations in the impedance response can be quantitatively ascribed to the changes in grain size or the precipitate population of the alloy or both.

9:55 AM Break

10:25 AM
Development of Functionally Graded Materials for Manufacturing Tools and Dies and Industrial Processing Equipment: Stanley M. Howard[1]; *Sudip Bhattacharya*[1]; James W. Sears[2]; [1]South Dakota School of Mines and Technology, Dept. of Matls. & Metallurgl. Engrg., 501 E. St. Joseph St., Rapid City, SD 57701 USA; [2]South Dakota School of Mines and Technology, Advd. Matls. Procg. Ctr., Rapid City, SD 57701 USA

The goal of this investigation was to produce improved dies for the metal casting, forging and glass forming industries by laser depositing functionally graded materials (FGM) on the working surfaces of the tools and dies. Typically, inexpensive H-13 or other grade tool steels are used for tools, dies and industrial process equipment, but they exhibit numerous failure modes including heat checking, soldering, fatigue, chipping and cracking, loss of hardness and corrosion. Longer wearing but prohibitively expensive materials are available for dies. In this work, the low cost of H-13 was combined with the high performance of expensive mold surfaces. The major features of interest in the graded materials are near-net shape, surface durability, and surface finishing. The FGM surfaces were produced using a laser powder deposition system employing a 3 KW Nd:YAG laser.

10:45 AM
Oxidation Resistance of Titanium Aluminides and Nickel Aluminides Intermetallic Compound Coatings on Inconel 738: *M. Reza Bateni*[1]; Morteza Zandrahimi[2]; Jerzy A. Szpunar[1]; [1]McGill University, Mining, Metals & Matls., 3610 Univ. St., M. H. Wong Bldg., Montreal, Quebec H3A2B2 Canada; [2]Shahidbahounar University, Engrg. Dept., Matls. Engrg. Grp., Jomhourieslami Bolv., Kerman Iran

In this research, attempts have been made to develop Al-Ti and Ni-Al intermetallic compound coatings on the surface of Inconel 738. The coatings were applied through pack cementation and simultaneous diffusion annealing processes. Scanning-electron microscopy

(SEM), energy-dispersive X-ray spectrometry (EDS), thermal gravimetric analysis (TGA) and grazing angle X-ray diffraction were used for evaluating the coating. It was demonstrated that the pack cementation technique could be used to develop TiAl3 and AlNi intermetallic compounds coating on Inconel 738 substrate. When pack cementation technique is based on a halide-activated pack with aluminum and titanium powders, the coating consists of TiAl3 intermetallic compound phase. Whereas, by pack aluminization of Inconel 738, the coating consists of AlNi intermetallic compound phase. It has found that the presence of intermetallic compound coatings on the surface, increase the oxidation resistance and the loss of elements from the protective coating, replenished by the interior layers, through interdiffusion.

11:05 AM
The Influence of Boron/Carbon Alloying on the Corrosion Behavior of NiSi19Nb3 Superalloy: Dong-Yih Lin[1]; Jen-Shen Hsu[1]; Shau-Shan Yen[1]; *Shian-Ching Jason Jang*[1]; Chen-Ming Kuo[2]; Shih-Jeh Wu[2]; [1]I-Shou University, Dept. of Matls. Sci. & Engrg., 1, Sec. 1, Hsueh-Cheng Rd., Ta-Hsu, Kaohsiung 84008 Taiwan; [2]I-Shou University, Dept. of Mechl. Engrg., 1, Sec. 1, Hsueh-Cheng Rd., Ta-Hsu, Kaohsiung 84008 Taiwan

NiSi19Nb3 superalloy due to its excellent mechanical properties and corrosion resistance usually is used as aerospace material. Parallel to the improving effect on the mechanical properties by alloying with boron and carbon in this material, its corrosion behavior is also interested for the further research. NiSi19Nb3 superalloy was melt doped with distinguished boron/carbon contents. Test materials were at 1080ºC for 4 hours solid solution and then at 700ºC for 10 hours aging treated. Various precipitates of test materials make their corrosion behavior noticeable difference that was studied according to the potentiostate (Perkin Elmer-263A) and their weight deviation. The microstructures of test materials and the precipitates in it were investigated via OM, SEM, EPMA and TEM. Some eutectic precipitates were observed obviously. Their influence on the corrosion behavior was studied in detail accordingly.

11:25 AM
Microstructural Evolution of Ni3Al Base Alloy IC6 and NiCoCrAlY Overlay Coating During Long Term Aero-Engine Test: *Yafang Han*[1]; Jinxia Song[1]; Shusuo Li[2]; [1]Beijing Institute of Aeronautical Materials, PO Box 81, Beijing 100095 China; [2]Beijing University of Aeronautics and Astronautics, Sch. of Matls., Xueyuan Rd. 37, Beijing 100083 China

The turbine vanes made of Ni3Al base alloy IC6 with NiCoCrAlY overlay coating were undergone engine test for 387h. The change of surface morphology and microstructure of both the substrate alloy and coating during the engine test has been studied. The results showed that there were no obvious microstructure change for the substrate alloy, and the NiCoCrAlY overlay coating were basically complete and still had certain oxidation and corrosion resistance, i.e., there was still a dense oxide layer mainly composed of Al2O3 on the surface although some black spots with various sizes appeared on the coating surface. The further analysis indicated that the contents of C, Na and Ca elements in the black spots area were higher than normal area without spots, suggesting that the formation of these black spots may resulted from the local corrosion and oxidation due to the agglomeration of the oil burning remants.

11:45 AM
Unusual Dislocation Density Oscillations After Local Melting and Solidification of Ni-Based Superalloys: *Oleg Barabash*[1]; S. S. Babu[1]; J. M. Vitek[1]; S. A. David[1]; G. E. Ice[1]; R. I. Barabash[1]; [1]Oak Ridge National Laboratory, Metals & Ceram., One Bethel Valley Rd., MS 6118, Oak Ridge, TN 37831-6118 USA

We studied how the dislocation structure of a Ni-based single crystal superalloy changes after melting and solidification. In our study, we combined polychromatic microbeam synchrotron diffraction measurements together with OIM, scanning electron and optical microscopy. We show that the distribution of the thermal gradient is not monotonic. Periodic dislocation structure is formed during continuous movement of melt zone in thin Ni-based superalloys sheet. Moreover we observe oscillations in the dislocation structure formed under such conditions at both macro and micro scales. Depending on the temperature, the formation of dislocations is accompanied by the partial or complete dissolution of ?×' particles in the matrix. Dislocations form and multiply due to thermal gradients. Their arrangement correlates with the temperature gradient field and with the dissolution and re-precipitation of ?×' particles. The distribution of the dislocation density at the macroscale is due to symmetric temperature gradient perpen dicular to the direction of melt zone movement. Within the above macro regions of dislocations oscillations of dislocation density due to grouping at the micro scale were also observed. Typical length scale of dislocation density oscillations is related to the dendrite size and the conditions of local melt and solidification.

Surface Engineering in Materials Science - III: Coating Properties and Processing Effects

Sponsored by: Materials Processing and Manufacturing Division, MPMD-Surface Engineering Committee
Program Organizers: Arvind Agarwal, Florida International University, Department of Mechanical and Materials Engineering, Miami, FL 33174 USA; Craig Blue, Oak Ridge National Laboratory, Materials Processing Group, Metals and Ceramic Division, Oak Ridge, TN 37831 USA; Narendra B. Dahotre, University of Tennessee, Department of Materials Science & Engineering, Knoxville, TN 37932 USA; John J. Moore, Colorado School of Mines, Department of Metallurgy and Materials Engineering, Golden, CO 80401 USA; Sudipta Seal, University of Central Florida, Advanced Materials Processing and Analysis Center and Mechanical, Materials and Aerospace Engineering, Oviedo, FL 32765-7962 USA

Thursday AM Room: 2022
February 17, 2005 Location: Moscone West Convention Center

Session Chairs: Lalgudi V. Ramanathan, Cidade Universitaria, IPEN/Matls. Sci. & Tech., São Paulo, 05508-000 Brazil; Arvind Agarwal, Florida International University, Dept. of Mechl. & Matls. Engrg., Miami, FL 33174 USA

8:30 AM
How Clean is Clean? Defining Acceptable Cleanliness Levels: *Mantosh Kumar Chawla*[1]; [1]Photo Emission Tech, Inc., 3255 Grande Vista Dr., Newbury Park, CA 91320 USA

A key to surface finishing is a "properly" prepared surface. Defining and maintaining the surface preparation at "proper" levels is at best subjective. Often the failure of surface preparation processes is not discovered until problems, such as poor adhesion, occur down stream resulting in non-conformance due to poor surface cleanliness. To assure consistent quality of surface cleanliness, one must not only specify an acceptable level of surface cleanliness but also specify a method for cleanliness monitoring. This generally leads to the question, what do we mean by "clean"? How clean is "clean"? This paper will discuss various methods available for monitoring surface cleanliness, their advantages and disadvantages, criteria for selecting an appropriate technique, approaches to establishing an acceptable level of cleanliness including optimum cost approach and introduce Optically Stimulated Electron Emission (OSEE) for quantitatively measuring surface cleanliness. Some typical OSEE application results will also be discussed.

8:45 AM
Vaporization Behavior of Solid Metal Carbonyls: *Dhanesh Chandra*[1]; Wen-Ming Chien[1]; Kai H. Lau[2]; [1]University of Nevada, Metallurgl. & Matls. Engrg., MS 388, Reno, NV 89557 USA; [2]SRI International, Menlo Park, CA 94025 USA

Carbonyls are generally used for CVD applications of high purity metal and alloy film formation at low temperatures. For these applications vaporization thermodynamics behavior of carbonyls is important. In this study, we have measured vapor pressures of low and high (>400 g/mol) molecular weight (MW) carbonyls using gravimetric-torsion effusion method. We will present results on Os3(CO)12, Rh6(CO)16, Ru3(CO)12, Re2(CO)10, Ir4(CO)12, Co2(CO)8, Cr(CO)6, and W(CO)6 carbonyls. There is propensity for disproportionation of solid carbonyls during heating, and it was virtually independent of molecular weight of the species. Vaporization studies of Rh6(CO)16 showed complete decomposition to nano-structured porous metallic Rh metal; the measured MWRh6(CO)16(effusing gas) is 27.75 g/mol was close to that of carbon monoxide as compared to MWRh6(CO)16(solid) of 1065.56 g/mol for the value of solid Rh6(CO)16. However, Ru3(CO)12 and Co2(CO)8 show very complex behavior. The total vapor pressures of all the above mentioned carbonyls, partial pressures of various species, average molecular weights of the effusing gases, equilibrium constants for the vaporization reactions, their enthalpies, entropies, and Gibbs energies have been determined.

9:00 AM
Understanding the Relationship Between Surfactant Adsorption and Metal Corrosion Inhibition: *Michael L. Free*[1]; [1]University of Utah, Metallurgl. Engrg., 135 S. 1460 E., Rm. 412, Salt Lake City, UT 84112 USA

Surfactants can be used as effective corrosion inhibitors in many industrial settings. This study examines the relationship between surfactant adsorption and corrosion inhibition as well as the factors that affect surfactant adsorption.

9:15 AM
The Thickness Uniformity of Films Deposited by Multi-Workpiece Magnetron Sputtering: Fu Chun Lin[1]; Yang Chuan Ren[1]; [1]University of Electronic Science & Technology of China, Inst. of Microelect. & Solid State Elect., Chengdu, Sichuan 610054 China

In this paper, a new radio frequency (RF) magnetron sputtering system with six workpiece and rotation and revolution was presented. A formula on the relation between the thickness of thin film and the parameters, such as rotation speed, revolution speed and the distance from target to substrate, was obtained. According to the formula, the three-dimensional curves of film thickness versus the parameters were drawn. From the curves, the optimum parameters of the system can be easily obtained for preparing uniform films or depositing films rapidly. It is found that the maximum relative deviation of film thickness distribution is less than 6% within a diameter of 4 inches when the ratio of the rotation speed to revolution speed is 5.3 and the results show good agreement with experimental ones.

9:30 AM
The Effect of Post-Annealing on the Structure of Barium Strontium Titanate Films Deposited by Radio Frequency Magnetron Sputtering: Liao Jiaxuan[1]; Yang Chuanren[1]; *Chen Hongwei*[1]; Fu Chunlin[1]; Leng Wenjian[1]; Zhao Li[1]; Gao Zhiqiang[1]; [1]University of Electronic Science and Technology of China, Sch. of Microelect. & Solid-State Elect., Chengdu 610054 China

Barium strontium titanate (BST) films were deposited on Pt/Ti/SiO2/Si substrate by radio frequency magnetron sputtering. Effects of post-annealing parameters on the structure of the as-deposited films have been investigated. It is found that a critical annealing temperature of approximately 500°C corresponds to the appearance of crystallization, resulting in an increase of roughness obtained by AFM. When temperature increases to 600°C, the crystallization is almost completed. AFM shows that each crystal grain grows uniformly and is 20-30nm in size, causing relatively smooth and dense morphologies. When temperature further increases, the grains become larger, thus the roughness increases. Also, annealing time has similar effect on the structure. Moreover, rapid thermal annealing in oxygen ambient can obtain much smoother and denser crystallization structure. The effects of other annealing parameters on the structure are also presented.

9:45 AM
Modeling the Effectiveness of Surfactants in Sub-Micron Particle Removal from Solid Substrates: *Michael L. Free*[1]; [1]University of Utah, Metallurgl. Engrg., 135 S. 1460 E., Rm. 412, Salt Lake City, UT 84112 USA

Surfactants can enhance the removal of sub-micron particles from critical substrates such as silicon wafers and optical lenses by orders of magnitude. This study shows how the adsorption of surfactant can be used to predict cleaning performance as well as techniques to predict surfactant adsorption as a function of ionic strength and surfactant hydrocarbon chain length.

10:00 AM Break

10:15 AM
Microstructured Electrode Arrays for Thin Film Deposition: *Nina Lucas*[1]; Philipp Sichler[1]; Christian Schrader[2]; Lutz Baars-Hibbe[2]; Stephanus Büttgenbach[1]; Karl-Heinz Gericke[2]; [1]TU Braunschweig, Inst. für Mikrotechnik, Alte Salzdahlumer Straße 203, Braunschweig 38124 Germany; [2]TU Braunschweig, Institut für Physikalische und Theoretische Chemie, Hans-Sommer-Straße 10, Braunschweig 38106 Germany

Non-thermal plasma processing techniques have been established for a wide range of applications. Microstructured Electrode (MSE) arrays are a new plasma source for generation of non-thermal plasmas. They allow to generate large-area uniform glow discharges over a wide pressure range up to atmospheric pressure. The electrode dimensions in the µm-range are realized by photolithography and galvanic techniques. They are small enough to generate sufficiently high electric field strengths to ignite gas discharges applying only moderate radio frequency voltages (RF, 13.56 MHz, 80 V to 390 V in Ne, He, Ar and N2). One area of application for non-thermal plasma processing is thin film deposition. With the MSE arrays as plasma source some applications in the field of thin film deposition (e.g. SiO2 layers on various substrates, DLC layers) were developed and successfully tested. Another atmospheric pressure application is the sterilization of food packaging materials.

10:30 AM
An Investigation of the Adhesion and Material Transfer Phenomena Between Al, Cu, Mg, Ti Metals and CrN, DLC, TiB_2 Coatings: *Erkan Konca*[1]; Yang T. Cheng[2]; Anita M. Weiner[2]; Ahmet T. Alpas[1]; [1]University of Windsor, Mechl., Auto. & Matls. Engrg. Dept., 401 Sunset Ave., Windsor, Ontario N9B 3P4 Canada; [2]General Motors R&D Center, Matls. & Processes Lab., 30500 Mound Rd., Warren, MI 48090 USA

This project has been initiated to study the relative contributions of the intrinsic and extrinsic factors that influence the adhesion and material transfer between some metals and coatings of interest to automotive industry. Rounded pins of Al, Cu, Mg and Ti were run against DLC, TiB_2 and CrN coated and uncoated M2 tool steel discs under dry sliding conditions. Tests were done under different sliding speeds (0.1-1 m/s), applied loads (1-10 N) and environments (Argon and air with various %RH). Sliding distances were kept short to focus on the initial stages of sliding. Sliding speed significantly influenced the degree of material transfer. The chemical affinity of the metal pins for oxidation, properties their oxides and interactions with the coatings had profound effects on the adhesion behavior. Here, the results of the tests performed under various conditions are explained in terms of the physical and chemical properties of the materials tested.

The Armen G. Khachaturyan Symposium on Phase Transformation and Microstructural Evolution in Crystalline Solids: Session VII

Sponsored by: Electronic, Magnetic & Photonic Materials Division, Materials Processing & Manufacturing Division, EMPMD/SMD-Chemistry & Physics of Materials Committee, MPMD-Computational Materials Science & Engineering-(Jt. ASM-MSCTS), MPMD-Phase Transformations Committee-(Jt. ASM-MSCTS)
Program Organizers: Yunzhi Wang, Ohio State University, Department of Materials Science and Engineering, Columbus, OH 43210 USA; Long-Qing Chen, Pennsylvania State University, Materials Science and Engineering Department, University Park, PA 16802-5005 USA; John William Morris, University of California, Department of Materials Science and Engineering, Berkeley, CA 94720 USA

Thursday AM — Room: 3003
February 17, 2005 — Location: Moscone West Convention Center

Session Chairs: Alan J. Ardell, University of California, MSE, Los Angeles, CA 90095 USA; David N. Seidman, Northwestern University, MSE, Evanston, IL 60208 USA

8:30 AM Opening Remarks

8:35 AM Invited
Atomic-Scale Dynamics of Transformation Interfaces: *James M. Howe*[1]; [1]University of Virginia, Dept. of Matls. Sci. & Engrg., 116 Engr.'s Way, Charlottesville, VA 22904-4745 USA

Frame-by-frame analyses of in-situ heating HRTEM experiments were preformed to determine the dynamics of a diffuse order-disorder interface and a sharp massive-transformation interface. The diffuse interface between ordered AuCu I and disordered alpha phases in Au-41at.%Cu alloy nanoparticles was studied at 305°C. Both the thickness and average position of the interface were found to vary with time. The disordered alpha side of the interface fluctuates more rapidly and over greater distances than the ordered AuCu I side. Frame-by-frame analyses of a moving high-index incoherent massive-transformation interface in Ti-46.5at.%Al alloy at 575°C show that the interface displays dynamic fluctuations in its trace that can be described in terms of a wave-like function with a characteristic amplitude and fundamental wavelength. The interface moves forward by the spreading of critical-size fluctuations along its length. This research was supported by NSF under Grant DMR-9908855.

9:00 AM Invited
Atomistic Modeling of Crystal-to-Amorphous Transition and Calculation of the Glass-Forming Ranges for Some Miscible/

Immiscible Binary Metal Systems: *Baixin Liu*[1]; [1]Tsinghua University, Dept. of MS&E, Beijing 100084 China

A brief review is presented to show that ion beam mixing and solid-state reaction of metal-metal multilayers are capable of producing amorphous alloys (metallic glasses) not only in miscible but also in immiscible systems within much broader composition ranges than those revealed by liquid melt quenching. In atomistic modeling, n-body potentials are derived for some miscible systems by routine methods and for some immiscible systems, where exists no any equilibrium alloy, by fitting their cross potentials to some physical properties acquired by first principles calculations. Based on the derived potential of a system, molecular dynamics simulations using solid solution models clarify that the physical origin of crystal-to-amorphous transition is crystalline lattice collapsing while solute atoms exceeding the two critical solid solubilities, between which the composition range is thus the intrinsic glass-forming range of the system. The simulation results are in excellent agreement with experimental observations.

9:25 AM

Semi-Empirical Atomistic Simulations for Energy and Structure Evolution on Surfaces or Grain Boundaries: *Byeong-Joo Lee*[1]; [1]Pohang University of Science and Technology, Dept. of Matls. Sci. & Engrg., Pohang 790-784 Korea

Surface energy or grain boundary energy, especially its orientation anisotropy, gives great effects on microstructural evolution and eventually on the materials properties of structural materials. Knowing the grain boundary energy and its anisotropy is essential for obtaining more realistic results through microscale simulation techniques. The surface or grain boundary structural transition is another important factor that should be considered in computational approaches. In the present study, a new atomistic computation method of grain boundary energy for arbitrary misorientations will be presented. It will also be presented that the structural transition on metallic surfaces and effect of alloying on the transition can be investigated by atomistic simulations based on semi-empirical interatomic potentials (MEAM).

9:40 AM

Microstructural Evolution Via Planar Interface Migration in Nanocrystalline Ni: *Glenn Hibbard*[1]; [1]University of Toronto, Dept. of Matls. Sci. & Engrg., 184 College St., Toronto, Ontario M5S 3E4 Canada

Microstructural evolution in nanocrystalline Ni occurs through multiple grain growth sequences. A distinctly unusual stage occurs after an initial sequence of abnormal grain growth followed by normal grain growth, in which a planar discontinuous growth interface migrates into a matrix of submicron-scale grains. This planar interface is one face of a highly symmetrically (typically cubic) growing grain. This growth morphology has been characterized by conventional transmission electron microscopy (TEM), scanning transmission electron microscopy (STEM) with energy dispersive X-ray spectroscopy (EDS), and scanning electron microscopy (SEM) with orientation imaging microscopy (OIM). Several interesting features are noted including, grain embedding for certain matrix grains having a low-sigma relationship with the discontinuously growing grain, and the presence of a wetting, sulfur-rich second phase at the planar growth interface.

9:55 AM

Non-Congruent Phase Transitions of S3 Grain Boundaries in Gold: *Tamara Radetic*[1]; Ulrich Dahmen[1]; [1]Lawrence Berkeley National Laboratory, NCEM, 1 Cyclotron Rd., MS 150, Berkeley, CA 94720 USA

Au mazed bicrystal thin films were grown on germanium substrates in order to study the stability of different inclinations of S3 <111> tilt grain boundaries in gold. In as- deposited thin films, single phase smoothly curved grain boundaries were observed, but the majority of boundaries exhibit two phase structure consisting of {112} facets. In-situ heating experiments confirmed expectations that the fraction of faceted boundaries increases during annealing. At temperatures above 900°C, prior studies have shown that roughening/defaceting transition takes place, transforming two-phase faceted grain boundaries into continuously curved single phase boundaries. However, we discovered that in the presence of Ge, roughening transition occurs at temperatures as low as 225°C. This paper reports the effect of Ge on the structure of grain boundaries, discusses the thermodynamics and kinetic limitations of the observed roughening transition. In addition the implications of defaceting at low temperatures on the properties of grain boundaries such as mobility and coarsening rates are also addressed.

10:10 AM Break

10:35 AM Invited

Prediction of Phase Transformations in Titanium Alloys - Different Modelling Approaches: *Elisabeth Marie Aeby-Gautier*[1]; B. Appolaire[1]; L. Héricher[1]; J. Da Costa Teixeira[1]; B. Antoine[1]; [1]Ecole des Mines, LSG2M CNRS UMR 7484, Parc de Saurupt, Nancy 54042 France

The study and modelling of successive and competitive phase transformations of hexagonal a phase from BCC high temperature b phase is considered for metastable multi component titanium alloys. To describe the transformation kinetics in a representative volume element, an analytical approach is considered for which nucleation and growth of grain boundary a phase is formed and in a second step colonies of a platelets nucleated from the a layer and grow inside the grain. A distribution of 1000 grains is considered whose grain boundary energy varies, leading to a distribution in nucleation rate. The growth of the a phase is described considering a local equilibrium at the interface for both layers and platelets. A given criteria allows nucleation of a platelets. This description allows to take into account the influence of a previous plastic deformation. In addition two models (a model with sharp interface and one with diffuse interface (phase field model) were developed to analyse, valid, test the limits of the analytical models and even improve it. Results obtained using these three approaches will be given and compared with experimental ones.

11:00 AM

Aspects of the Microstructural Evolution in Titanium Alloys: Sujoy Kar[1]; *Rajarshi Banerjee*[1]; Eunha Lee[1]; Gopal Babu Viswanathan[1]; Hamish L. Fraser[1]; [1]Ohio State University, Matls. Sci. & Engrg., 477 Watts Hall, 2041 College Rd., Columbus, OH 43210 USA

The solid-state beta to beta + alpha transformation in titanium alloys leads to rather interesting microstructures with features spanning across a range of length scales. Consequently, in order to understand the property-microstructure relationships in these alloys a detailed understanding of microstructural evolution is imperative. A series of controlled heat-treatments have been performed on alpha + beta Ti alloys with the objective of arresting the microstructure at successive stages of development. The crystallography of the microstructure has been studied in detail by employing orientation imaging microscopy (in a high resolution SEM), site-specific TEM sample preparation using focused ion beam, and subsequent TEM characterization. The influence of variant selection on the evolution of microstructure and the resulting development of the colony (clustering of the same variant) and basketweave (clustering of multiple variants) microstructures in these alloys will be specifically addressed in this presentation.

11:15 AM

Modelling the Local and Effective Behavior of Viscoplastic Polycrystals Using Fast Fourier Transforms: *Ricardo A. Lebensohn*[1]; [1]Los Alamos National Laboratory, MST-8, MS G755, Los Alamos, NM 87545 USA

We present some new applications of a novel and very efficient approach[1] that makes use of the Fast Fourier Transform (FFT) algorithm to obtain the intracrystalline fields and the effective response of anisotropic viscoplastic (nonlinear) polycrystals, based on the solution of a unit-cell problem for a representative volume element with periodic boundary conditions. This approach provides an exact solution of the equilibrium equation and has better numerical performance than a FE analysis of the same problem. The FFT model is used to predict local states and morphologic and crystallographic texture evolution of fcc polycrystals, as well as to obtain the effective behavior and the average field fluctuations in statistically random fcc and hcp polycrystals, for comparison with various estimates of the self-consistent type. [1]Michel, J., Moulinec, H. & Suquet P., 2000, Comput. Modelling Engng. Sc. 1, 79.

11:30 AM

The Evolution Constitution and Microstructure During Hot-Working of Titanium Aluminide Alloys: *Michael Oehring*[1]; Lorenz Uwe[1]; Fritz Appel[1]; [1]GKSS Research Centre, Inst. for Matls. Rsch., Geesthacht D-21502 Germany

Titanium aluminide alloys containing relatively large Nb additions and subjected to precipitation hardening exhibit attractive thermophysical properties, which extend the service range of conventional TiAl alloys. In order to use these materials at their full potential, structural and chemical consolidation is required. To this end, the feasibility of wrought processing of high Nb containing alloys was systematically investigated. The major areas of the study involve: (i) high-temperature deformation mechanisms, (ii) primary ingot breakdown, (iii) secondary processing, (iv) texture evolution, and (v) me-

chanical properties. The experimental investigation base on standard metallography, chemical microanalysis, mechanical testing, and high-resoltuin electrom microscopy.

11:45 AM
Initiation of Adiabatic Shear Localization in a Pre-Shocked 304 Stainless Steel: *Qing Xue*[1]; Benjamin L. Henrie[1]; George T. Gray[1]; [1]Los Alamos National Laboratory, Matls. Sci. & Tech. Div., G755, Los Alamos, NM 87545 USA

Initiation of adiabatic shear bands in a pre-shocked stainless steel was studied to characterize the influence of prestrained texture on the onset of shear bands. Forced shear tests on hat shaped specimens was conducted using a compressive Hopkinson bar to generate shear localization. The initiation of adiabatic shear localization was found to be very sensitive to the prestrained texture, especially to distribution of defects such as deformation twins. The variation of microstructure before and during the formation of shear bands was examined and compared. Twin orientation due to the prestraining was seen to exert a significant effect on triggering the nucleation of a shear band. Multiple microbands were observed to align perpendicular to the shear direction prior to the formation of shear localization. Transmission electron microscopy was applied to identify the microstructure inside and in front of shear bands.

Notes