

such as bond strength, tightness of core powder and rolling defect, the best reduction should be controlled at 60%~70%. The compound board can get the perfect foam structure under proper foaming technology: the best foaming temperature is 620~640°C; foaming time is 8~10min. Both intermetallic compound of FeAl₃ and Fe/Al solid solution with about 10µm thickness occur at the interface after foaming.

10:00 AM

FeAl-Based Intermetallic Sinters Obtained by Liquid Phase Sintering: Stanislaw Józwiak¹; Krzysztof Karczewski¹; Zbigniew Bojar¹; ¹Military University of Technology

The results of the optimization process of liquid phase sintering of Fe and Al powders in order to fabricate FeAl intermetallic sinters were studied in this paper. The oxidation of Al particles in the sintering process is responsible for the formation of the Al₂O₃ films in the sintered structure that are mainly located on the interparticle boundaries, which eventually lead to the decrease of the strength of material. The exothermic reaction of the mixed Fe +Al powders (SHS) may lead to the destruction of the sinter. Control of the process parameters such as pressure, temperature and time allowed fabrication of sound FeAl sinters by eliminating such adverse effects as strong oxidation of aluminum powder, self-propagating synthesis and resulting high porosity. The proposed three-stage technological process of fabricating FeAl intermetallic alloys from pure Fe and Al elemental powders which utilizes sintering with liquid phase allows us to obtain a fine-grained material.

10:20 AM Break**10:40 AM Invited**

Characterization of Particle Reinforced Metal Matrix Composite Microstructures by Three Dimensional (3D) Finite Body Tessellation: Jason Williams¹; Nikhilesh Chawla¹; ¹Arizona State University

The degree of clustering of particles has a significant influence on the mechanical behavior of particle reinforced metal matrix composites (MMCs). The clustered particles act as crack initiation sites and generally have a negative effect on tensile strength, ductility, toughness, and fatigue strength of the composite. Quantifying the degree of clustering in MMCs and other heterogeneous systems is a challenge. In this presentation we report on a novel, 3D finite-body tessellation scheme for quantifying the degree of clustering in SiC particle reinforced Al matrix composites. The results were compared to 2D representations and the salient differences will be highlighted. A methodology for correlating degree of clustering and mechanical properties of the composite will be discussed.

11:00 AM

Microstructure and Adhesion Strength of the Sn-9Zn-1.5Ag-1.5Bi Solder Alloy on Cu Substrate: Chih-Yao Liu¹; Moo-Chin Wang²; Min-Hsiung Hon¹; ¹National Cheng Kung University; ²National Kaohsiung University of Applied Sciences

The microstructure and adhesion strength between the Sn-9Zn-1.5Ag-1.5Bi and Cu substrate has been investigated. The Sn-9Zn-1.5Ag was also tested for comparison. The phase formation observed in two solders by an X-ray diffractometer (XRD), an scanning electron microscope (SEM), an energy dispersive spectrometer (EDS) and a transmission electron microscope (TEM). The adhesion strength was 8.34 ± 0.28 for Sn-9Zn-1.5Ag-1.5Bi. Fracture morphology were revealed that the fracture occurred in solder matrix by scanning electron microscopy. The intermetallic compounds Cu₆Sn₅ and Cu₅Zn₈ were observed in the Sn-9Zn-1.5Ag and Sn-9Zn-1.5Ag-1.5Bi solder alloy. After 150°C with 1000 hour aging, the adhesion strength was decreased to 3.48 ± 0.63 MPa because of the growth and decomposition intermetallic compounds.

11:20 AM

Atomic Level Characterization of the β Decomposition Products in Ti-6Al-4V Using the Local Electrode Atom Probe: Stephanie Johnson¹; David Diercks¹; Rajarshi Banerjee¹; James Cotton²; Michael Kaufman¹; ¹University of North Texas; ²Boeing Company

Upon cooling from above the β transus, Ti-6Al-4V undergoes a transition from BCC to HCP by a martensitic transformation at high cooling rates and by nucleation and growth at slower rates. The transition from one mechanism to the other as a function of cooling rate remains controversial as does the mechanism in which a cubic phase shears to form a higher-symmetry HCP

phase. In this study, a Ti-6Al-4V sample was subjected to a modified Jominy end quench test in order to produce a range of cooling rates. Both TEM and 3-D atom probe tomography were used to analyze the sample at atomic resolution. The results will be discussed in terms of the light they shed on transformations in this class of titanium alloys. *Characterization performed using analytical facilities in the Center for Advanced Research and Technology at the University of North Texas. Partial support of The Boeing Company is appreciated.*

11:40 AM

Thermal Properties of the Diamond-Copper Interface in Hot-Pressed Metal-Matrix-Composites: Ivica Smid¹; Erich Neubauer²; Paul Angerer³; Kristina Cowan¹; ¹Pennsylvania State University; ²Austrian Research Centers; ³ECHEM

Copper Metal-Matrix-Composites (MMCs) based on carbon reinforcements have a high potential for application as heat sink material. Basically the thermal properties can be tailored by a simple variation of the volume fraction of the reinforcement. Another important parameter for achieving a high conductivity in the copper-carbon system is the thermal contact resistance (TCR). By a variation of the TCR the whole range between an insulating interface and a perfect heat transfer can be simulated. The experimental values of the TCR were determined by photothermal methods. The resulting bulk thermal properties have been modeled using finite element methods, allowing a prediction of the maximum achievable conductivity as a function of composition and processing. Filler particle size and shape limitations in view of bulk conductivity requirements have been determined.

12:00 PM

Processing of Nanocrystalline and Amorphous Fe-(Co)-B-Si Thin Wires for Magnetic Applications by Using in-Rotating-Liquid-Spinning: Georg Frommeyer¹; Joachim Gnauk¹; Susanne Zeller¹; ¹Max-Planck-Institut für Eisenforschung

A computer controlled facility for continuous casting of metallic thin wires performing inrotating-liquid-spinning (INROLISP) was designed and installed to determine and control the near-net-shape casting process over an extended time period. In particular, the flow of the melt was experimentally investigated and theoretically described using fluid dynamic equations. The controlling process parameters, such as the velocity of the melt jet, the stable free flight length, the nozzle geometry and cooling rate were examined and optimized. Several pure metals as well as microcrystalline and amorphous alloys were cast into continuous wires of high quality. Microstructural features and mechanical properties of rapidly quenched fibres were evaluated. The production of softmagnetic amorphous and nanocrystalline FeSiB and CoFeSiB thin wires of 50 µm to 120 µm in diameter is an application of great potential. These microwires are used as sensor cores in highly sensitive magnetic field sensors, based on the magneto-electric Procopiu effect. The sensor properties determined by the alloy composition and the microstructure features, will be correlated with the process parameters.

Advances in Computational Materials Science and Engineering Methods: Methods at the Atom Scale I

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

Monday AM Room: Europe 7
February 26, 2007 Location: Dolphin Hotel

Session Chair: Richard LeSar, Iowa State University

9:00 AM Introductory Comments**9:05 AM Invited**

Molecular Dynamics Simulations of the Structure and Properties of Confined Amorphous Films in Ceramics: Stephen Garofalini¹; ¹Rutgers University

The structure of thin (O(nm)) amorphous films confined between crystals or within pores significantly modifies the structure of the film and the



resultant properties of the material. Two examples include thin glassy silicate intergranular films (IGFs) between oxide or nitride crystals and water confined within nanometer size pores. In the former, the composition and structure of the IGF can significantly modify grain growth and the mechanical properties of the polycrystalline ceramic. Results of molecular dynamics (MD) simulations of silicate films in alumina and silicon nitride showing preferential segregation of species from the IGF and the effect of composition on growth of specific orientations and strength will be presented. In the second case, MD simulations of confined water using a new dissociative water potential will also be presented. The new potential matches many experimental properties of bulk water and also newly obtained data regarding the anomalous expansion of confined water.

9:40 AM Question and Answer Period

9:45 AM

Diffusion-Limited Processes Treated with Accelerated Molecular Dynamics: *Erdi Bleda*¹; Murray Daw¹; ¹Clemson University

We treat diffusion-limited processes using Accelerated Molecular Dynamics. On-the-fly kinetic Monte Carlo is combined with the Dimer Method to find the saddlepoints exiting a valley, based on energetics from the Embedded Atom Method. With this technique, we treat two cases involving diffusion-limited processes in situations with very low symmetry. First, we calculate the tracer diffusivities in ordered intermetallics as a function of composition and temperature. We investigate both a strongly ordered case (Ni₃Al) and a less-strongly ordered case (Cu₃Au). In the latter, we investigate especially the diffusivity near the order-disorder transition. Second, we treat the motion of an anti-phase boundary (APB) in the same intermetallics. We demonstrate how an APB can be moved perpendicular to itself perpendicular to itself via vacancy motion. We conclude that the on-the-fly kMC is useful for investigating diffusivity in intermetallics. (The author acknowledges support from NSF.)

10:10 AM Question and Answer Period

10:15 AM

Linkage between Atomistic and Continuum-Based Simulations in Nanoscale Powder Metallurgy: Amitava Moitra¹; Sungho Kim¹; Seong-Gon Kim¹; Seong Jin Park¹; *Randall German*¹; ¹Mississippi State University

The atomistic and continuum-based simulations used in this paper are concerned with the multiscale computer modeling during sintering process of nanoscale powder. Of first interest is the application and development of classical and quantum mechanical methodologies to gain insight into the fundamental characteristics of atomic movement during nanoscale powder sintering and how they influence the sintering processing and the physical properties of the material such as melting temperature decrement, sintering activation energy, and so on. These predicted material properties may play a role as bridge between two different scale simulations. This paper focuses on the material properties related to densification predicted from atomistic simulation and their possibility to use in continuum-based simulation.

10:40 AM Question and Answer Period

10:45 AM Break

11:15 AM

Multiscale Modeling of Nanoindentation: Ed McGee¹; *Steven Kenny*¹; Roger Smith¹; ¹Loughborough University

We will present a 3D multiscale model of nanoindentation that couples a molecular dynamics (MD) model with a finite element (FE) model. The MD model is used to describe the tip and the material around the tip at the atomic scale, allowing for an accurate description of plastic deformation. The FE model is used to describe the long range elastic fields in the material. We will show how this model gives contact pressures which are in better agreement with experimental results than traditional atomistic only models, illustrating that a correct description of the long range elastic field is essential. Nanoindentation of the Au (100) surface using a second nearest neighbour embedded atom potential will be used to illustrate the methodology.

11:40 AM Question and Answer Period

11:45 AM

Topological Characterization of Adsorption Phenomena Using Multi-Body Potential Expansions: Nicholas Zabaraz¹; *Baskar Ganapathysubramanian*¹; ¹Cornell University

The enhancement of adsorption of (hydrogen) molecules on metallic surfaces is a key challenge for producing feasible fuel cell technologies. Along with the chemistry of the surface under consideration, the topology of the surface also plays an essential part in the adsorption phenomena. There exists a possibility to design both the material specification as well as the surface topology to further enhance the adsorption phenomena. In the present approach, long-ranged and many-body interactions are necessary to model the potential accurately. We construct many-body expansions from a large database of computed ab-initio energies which includes the interaction between the molecule and small clusters of the surface. Non-uniform surfaces are represented in terms of expanding cluster of atoms. Effects of small scale roughness and waviness of the surface on the adsorption are reported. An approach to design the topology of the surface to enhance adsorption based on optimization techniques is presented.

12:10 PM Question and Answer Period

12:15 PM

Development and Testing of MEAM Potential for Al-Mg Alloys: *Bohumir Jelinek*¹; Seong-Gon Kim¹; Jeffery Houze¹; Sungho Kim¹; Mark Horstemeyer¹; Michael Baskes²; ¹Mississippi State University; ²Los Alamos National Laboratory

A MEAM potential for Al-Mg alloys was developed based on the elastic and structural properties determined from ab-initio calculations. Transferability of the new potential was tested by comparing various bulk, surface, and point defect properties with ab-initio simulations. Volume-energy dependence of Al and Mg in fcc, hcp, bcc and simple cubic crystal structures from MEAM and ab-initio simulations was determined. Heat of formation for Al-Mg crystals in C1, C3, C9, C15, D0₃, D0₉, A12, A15, L1₂, B1, B2, and B3 was calculated using both methods. Surface formation, stacking faults, and adsorption energies were compared. For point defects calculations, a close agreement of vacancy formation energies, interstitial and substitutional point defect energies was found.

12:40 PM Question and Answer Period

Advances in Microstructure-Based Modeling and Characterization of Deformation Microstructures: Characterization of Deformed Structures I

Sponsored by: The Minerals, Metals and Materials Society, ASM-MSCTS: Texture and Anisotropy Committee, ASM-MSCTS: Texture and Anisotropy Committee

Program Organizers: Reza Shahbazian Yassar, Center for Advanced Vehicular Systems; Sean Agnew, University of Virginia; Jiantao Liu, Alcoa Technical Center

Monday AM
February 26, 2007

Room: Europe 1
Location: Dolphin Hotel

Session Chairs: Sean Agnew, University of Virginia; Anthony Rollett, Carnegie Mellon University

9:00 AM

Deformation-Induced Microstructural Development of Al-Base Sheet Metals: *Stephen Banovic*¹; Mark Iadicola¹; Tim Foecke¹; ¹National Institute of Standards and Technology

Reducing automotive vehicle weight by replacing conventional steel sheet metal with lightweight materials has been initiated. However, implementation of these lightweight alloys, specifically aluminum-base materials, has been slow due to both a limited knowledge of material behavior and a lack of experience in the sheet forming process. To obtain a better understanding of the material characteristics during in-plane stretching, the underlying microstructural development of aluminum alloy sheet metals was studied. Experimental characterization consisted of light optical microscopy, electron