



matrix of molybdenum solid-solution ( $Mo_{ss}$ ). However, bend testing of pure Mo and  $Mo_{ss}$  samples has shown that, while the powder processing route can produce ductile Mo metal, the hardening effect of Si and B in solid-solution renders the matrix brittle. Testing at elevated temperatures (200°C) was performed in order to determine the ductile-to-brittle transition temperature of the metal as an indication of ductility. Methods of ductilizing the  $Mo_{ss}$  matrix such as annealing and alloying additions have been investigated.

**11:20 AM**

**High Temperature Strength of Mo-Re-X Ternary Alloys:** *Joachim Schneibel*<sup>1</sup>; E. Felderman<sup>2</sup>; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>Arnold Engineering Development Center

Additions of Re to Mo improve the room-temperature ductility, but do not significantly increase the strength at elevated temperatures (e.g., 1700 K). In this work, the influence of ternary alloying elements such as Zr, Al, Ti, Nb, Ta, Cr, Hf, and Si on the high temperature compression strength of Mo-Re-X alloys was evaluated. Hafnium was found to be a particularly effective – 2 at% Hf approximately doubled the 1700 K yield strength of Mo-41 wt% Re. Also, Hf additions up to 2 at% reduced the tensile stress at which room temperature twinning occurred. The room temperature ductility of specimens prepared from cast and annealed Mo-Re and Mo-Re-Hf was only a few percent, but higher ductility values are expected with improved material and specimen preparation.

**11:40 AM**

**Improved Mechanical Properties of Ultrafine Grained Nb-1%Zr via Equal Channel Angular Extrusion (ECAE):** *Guney Yapici*<sup>1</sup>; Ibrahim Karaman<sup>1</sup>; Hans Maier<sup>2</sup>; <sup>1</sup>Texas A&M University; <sup>2</sup>University of Paderborn

Nb-1%Zr is widely used in a number of applications ranging from biomedical industry to space nuclear reactor concepts. Their relatively high operating temperature capability, chemical and biocompatibility and stability in nuclear environments make them attractive candidates over other alloy systems. In general, these applications require high strength and desired elastic modulus combined with enhanced ductility that Nb-1%Zr lacks in wrought condition. This talk will summarize our recent work on the ECAE of Nb-1%Zr for achieving target mechanical properties by engineering microstructure and crystallographic texture. Nb-1%Zr was processed up to 16 passes at room temperature without any shear localization. Post-processing of extruded billets with conventional forming techniques assisted by low temperature annealing treatments led to the formation of microstructures yielding both high tensile strengths and uniform strains (over 900 MPa and 20% ductility). Low cycle fatigue experiments showed stable response with improved cyclic stress range and number of cycles to failure.

**12:00 PM**

**Phosphide Precipitates in Copper-Based Alloys:** *Joon Hwan Choi*<sup>1</sup>; <sup>1</sup>Korea Institute of Machinery and Materials

Several types of copper-based alloys having phosphorus with one or more transition metals such as manganese, nickel and iron were designed to have high strength with good electrical conductivity. A study on aging characteristics of the Cu-TM-P (TM= Mn,Ni,Fe) alloys showed that the molar ratios between the total amount of the transition metals and phosphorus to obtain an optimum combination of mechanical and electrical properties were close to 2:1. TEM analysis revealed precipitate phases formed during aging had  $M_2P$  (M = Mn and/or Ni and/or Fe) formulation and their crystallographic structures depended on the type of the elements. TEM analysis also showed there existed orientation relationships between the precipitates and copper matrix in non-recrystallized regions of the alloys.

**12:20 PM**

**Comparison and Characterization of Copper-Graphite Composites Made with Cu-Coated and Uncoated Graphite Powders:** *Liu Wei*<sup>1</sup>; Yao Guangchun<sup>1</sup>; Liu Yihan<sup>1</sup>; <sup>1</sup>Northeastern University

Copper-graphite composites of graphite contents of 5, 10, 15, and 20 wt% made by powder metallurgy route using either Cu-coated graphite powders or mixture of copper and graphite powders. The Cu-coating process of graphite powders was carried out using electroless coating technique. Physical and mechanical properties, electrical conductivity, energy to fracture and wear behaviour, have been measured. It was found that composites made by Cu-coated and uncoated graphite have lower rates and friction coefficients than

those made from pure copper, and made by Cu-coated graphite have better mechanical properties than uncoated graphite. The technological conditions were also studied to determine the optimum conditions.

## Advances in Computational Materials Science and Engineering Methods: Phase Field Methods 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

Tuesday AM

Room: Europe 7

February 27, 2007

Location: Dolphin Hotel

*Session Chair:* Richard LeSar, Iowa State University

**9:00 AM Introductory Comments**

**9:05 AM Invited**

**Phase-Field Modeling of Solid State Phase Transformations and Microstructure Evolution:** *Long Qing Chen*<sup>1</sup>; <sup>1</sup>Pennsylvania State University

Many of the technologically important materials are designed by controlling their phase transformations and/or microstructure evolution. Examples include the improvement of mechanical properties through solid state precipitation reactions in alloys such as Ni-based superalloys and the useful dielectric properties and electro-mechanical coupling effects by manipulating the phase transitions in ferroelectric crystals. This presentation will briefly review the applications of phase-field method to solid state phase transformations and microstructure evolution. A number of recent advances will be highlighted, including nucleation in the presence of long-range elastic interactions, ferroic transitions and domain structures thin film and bulk crystals, and multiscale modeling of alloy microstructure evolution in complex alloys.

**9:40 AM Question and Answer Period**

**9:45 AM**

**A Comparative Study of Numerical Methods and Computational Tools for Phase Field Equations of Solidification:** *Zhiheng Huang*<sup>1</sup>; Paul Conway<sup>1</sup>; <sup>1</sup>Loughborough University

A Partial Differential Equation (PDE) or coupled PDEs need to be solved in phase field microstructural modelling. Finite difference discretization in space is commonly used to solve such equations numerically. Spectral methods can also solve PDEs to a high accuracy on a simple domain. However, those two methods should be treated with care when the domain of interest is irregular. In such cases, finite volume method or finite element method is a natural alternative. A numerical algorithm implemented in a basic computer language such as C normally runs fastest. However, some high level computing environments or software packages provide the advantages of easy implementation and flexibilities in visualization. This paper provides a comparative study of using different numerical methods and computational tools to solve coupled phase field equations of solidification. The methodologies presented in this paper can be equally applied to other PDEs in phase field modelling.

**10:10 AM Question and Answer Period**

**10:15 AM**

**A Level Set Simulation of Dendritic Solidification of Multi-Component Alloys:** *Nicholas Zabaravski*<sup>1</sup>; Lijian Tan<sup>1</sup>; <sup>1</sup>Cornell University

A level set method combining features of front tracking methods and fixed domain methods is presented to model microstructure evolution in the solidification of multi-component alloys. Phase boundaries are tracked by solving the multi-phase level set equations. Diffused interfaces are constructed from these tracked phase boundaries using the level set functions. Based on the assumed diffused interfaces, volume-averaging techniques are applied for energy, species and momentum transport. Microstructure evolution in multi-component alloy systems is predicted using realistic material parameters. Techniques including fast marching, narrow band computing and adaptive

meshing are utilized to speed up computations. Several numerical examples are considered to validate the method and examine its potential for three-dimensional solidification modeling of practical alloy systems.

#### 10:40 AM Question and Answer Period

#### 10:45 AM Break

#### 11:15 AM

#### Phase Field Modeling of Strained Heteroepitaxial Multilayer Thin Film Evolution: *Ramanarayan Hariharaputran*<sup>1</sup>; Vivek Shenoy<sup>1</sup>; <sup>1</sup>Brown University

Nanopatterns formed during multilayer growth by Asaro Tiller Grinfeld instability of strained/spacer layers or alternately strained layers are of current interest for their unique optical and electronic properties. Earlier theoretical studies were restricted to linear stability analysis to identify a phase stability diagram as a function of kinetic parameters with only surface diffusivity and simplified elastic state of the multilayer. Here, we present a new phase field model to simulate the non-linear evolution of strained multilayer growth. We observe three growth regimes namely, layered superlattice growth of alternate phases, aligned correlated islands and lateral composition modulation of the two phases which agree with experimental observations. We characterize our results in terms of kinetic parameters namely, deposition flux, surface and bulk diffusivities and material parameters like misfit strain and surface energies of the individual layers.

#### 11:40 AM Question and Answer Period

#### 11:45 AM

#### Multiscale Phase Field Modeling of Phase Transformations in Solids: *Valery Levitas*<sup>1</sup>; Dong-Wook Lee<sup>1</sup>; Dean Preston<sup>2</sup>; <sup>1</sup>Texas Tech University; <sup>2</sup>Los Alamos National Laboratory

The following basic problems of modeling of martensitic phase transformations based on the Ginzburg-Landau approach are discussed: 1. New thermodynamic potentials for stress-induced martensitic phase transformations, both for small and large strains. 2. Analytical solutions for one-dimensional spatial variation of the order parameter: various types of static microstructures, their stability and physical interpretation. 3. Phase transformations in nanosize sample: surface effect, new microstructures, new functionally graded nanophases, barrierless surface-induced nucleation. 4. Finite element modeling martensite nucleation at dislocations and microstructure formation. Alternative phase field modeling approach is developed for the scale from 100nm and without upper limit. Martensitic microstructure evolution in a single and polycrystalline sample under uniaxial loading is found using finite elements method.

#### 12:10 PM Question and Answer Period

#### 12:15 PM

#### Computing Property Variability of Polycrystals Induced by Grain Size and Orientation Uncertainties: *Nicholas Zabaras*<sup>1</sup>; *Sethuraman Sankaran*<sup>1</sup>; <sup>1</sup>Cornell University

Multiscale computational methods bridging models at micro scale with macro properties is a problem of practical significance since many macroscopic properties depend strongly on geometrical variability of the micro-constituents. Probability distribution functions (PDFs) providing a complete characterization of microstructural variability in polycrystalline materials using limited information is difficult to obtain since this inverse problem is highly ill-posed. We use the maximum entropy principle to compute a PDF of microstructures based on given information about a microstructural system. Microstructural features are incorporated into the maximum entropy framework by obtaining data either from experiments or simulations. Grain size features are here extracted from a set of representative microstructures using phase-field simulations. Microstructures are sampled from the computed PDF using concepts from computational geometry and voronoi-cell tessellations. These microstructures are then interrogated using homogenization techniques to evaluate the variability of non-linear macro properties.

#### 12:40 PM Question and Answer Period

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

*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

Tuesday AM Room: Europe 1  
February 27, 2007 Location: Dolphin Hotel

*Session Chairs:* Reza Shahbazian Yassar, Center for Advanced Vehicular Systems; Matthew Miller, Cornell University

#### 9:00 AM

#### Influence of the Interactions between Dislocation Mechanisms on Internal Strain Generation in HCP Zircaloy-2: *Feng Xu*<sup>1</sup>; Mark Daymond<sup>1</sup>; Rick Holt<sup>1</sup>; <sup>1</sup>Queen's University

Zircaloy2 is an hcp alloy, used in nuclear industries for core components, e.g. pressure tubes in heavy water reactors and fuel cladding in heavy and light water reactors. Intergranular strains in Zircaloy2 can greatly affect mechanical performance. It is thus important to know how the material responds on macro- and microscopic scales to different external loadings, and what deformation mechanisms lead to the observed responses. We have used neutron diffraction to determine the lattice strain development/texture changes when the material was subjected to either compression or tension, in three directions relative to a parent texture, and elasto-plastic self-consistent models to interpret the data. Model parameters describing the deformation were obtained through simultaneous fitting of all experimental flow curves and internal strain data. Assessment of the data set demonstrated the importance of incorporating hardening effects arising due to interaction between different dislocation mechanisms. Substantial tensile twinning was inferred from intensity changes.

#### 9:25 AM Invited

#### Measuring the Mechanical Response of Polycrystalline Alloys at the Crystal Level: *Matthew Miller*<sup>1</sup>; <sup>1</sup>Cornell University

While multiscale models are being employed more regularly, truly multiscale validation experiments are much less common. Using new in-situ mechanical loading / diffraction techniques and technologies, it is now possible to measure lattice strains and quantify stress on the crystal level in-situ using synchrotron x-ray diffraction. This talk describes an experimental system and approach developed at Cornell and employed at the Cornell High Energy Synchrotron Source (CHESS) and the Advance Photon Source (APS). This system was designed to load polycrystalline samples while conducting x-ray diffraction experiments. A 0.5mm x 0.5mm beam of 50-100 keV synchrotron x-rays is used to interrogate an aggregate of grains. While loaded, the sample stage is rotated and strain pole figures are constructed. Lattice strain distributions functions (LSDFs) and crystal stresses are then derived. In this manner, the three-dimensional response of the crystals can be ascertained. This talk describes recent work on two phase titanium alloys.

#### 9:50 AM

#### Application of the Artificial Intelligence Techniques in Modeling the Microstructure-Property Relationships of Materials: *Osama AbuOmar*<sup>1</sup>; Reza Shahbazian Yassar<sup>2</sup>; Eric Hansen<sup>3</sup>; Kyla Stoltzing<sup>4</sup>; <sup>1</sup>Computer Science Department; <sup>2</sup>Center for Advanced Vehicular Systems; <sup>3</sup>Mississippi State University; <sup>4</sup>Mechanical Engineering Department

The quantitative analysis of physically measured microstructural parameters plays an important role in establishing the microstructure-property relationship of materials. In the present research, various machine learning algorithms were used to establish the correlation between dislocation substructures and the materials' flow stress. Using Nye's dislocation density tensor, the densities of geometrically necessary dislocations were calculated and an algorithm was developed to extract the thickness of the dislocation (substructures) boundaries and the mean free path of the subcells. In the next