4:05 PM
Synthesis and Production of Ni-Mo Alloys for Hydrogen Production via Mechanical Alloying: *Maria Valero Rocha*[1]; Roberto Martinez Sanchez[1]; Jose Cruz Rivera[2]; Israel Rodriguez Torres[2]; [1]Centro de Investigacion en Materiales Avanzados, S.C.; [2]Instituto de Metalurgia

The present work studied the structural and microstructural evolution of Ni-Mo alloys (10%, 20% and 30%Wt) produced by Mechanical Alloying. Alloys production was performed in a commercial Fritsch planetary mill, the ball-to-powder weight ratio was 6:1, and the process control agent used was hexanos. Nominal compositions of original powders were 99.99% purity, the particle sizes was 2.23 µm and 67.93 µm, respectively. Mixtures of powders of Ni-10%Mo, Ni-20%Mo and Ni-30%Mo were milled by different times. After Milling, powders were cold compact. The sintering compacts were carried out in a resistance tubular furnace. Structural and morphological characterization of the powders and the sintering materials were performance by XRD, SEM, TEM and EDS. From characterization results it is possible to observe an increment in the parameter which suggests that during the process a solid solution and nanometric phase were formed. The results has been analyzing in cathodes for hydrogen production.

4:20 PM
Shape-Controlled Synthesis of Porous Fibrous Cobalt Powders: *Zhan Jing*[1]; Dong Chengyong[1]; Zhang Chuanfu[1]; Wu Jianhui[1]; Fan Youqi[1]; [1]Central South University

The fibrous precursor can be obtained by coordination precipitation process. The composition and morphology of fibrous precursor were characterized by XRD, IR, DTA/TGA and SEM analysis. The results show that XRD pattern and composition of the precursor with fibrous morphology precipitated at pH=9.0 are different from that of ß-CoC2O4•2H2O precipitated at pH=1.0. The mechanism on the thermal decomposition of fibrous precursor was addressed The influences of various conditions in pyrolysis, including the temperature, time, atmosphere, and the morphology of the precursor, on the morphology, average size and specific surface area of the Co powders were investigated in detailed. At last, the final product-fibrous cobalt powders with about 0.3~0.5µm in size and 40~60 in aspect ratio were produced by thermal decomposition at 400~500° in the weak reducing atmosphere. The structure of pores in cobalt powders is capillary tube with open ports and the majority is mesoporous.

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Synthesis of Nanometer Core-shelled Titanium Dioxide/Tungsten Oxide Powder: *Daoxin Wu*[1]; [1]Changsha University of Science and Technology

With the controllability in composition,structure and property,the complex core-shelled nanoparticles have attracted both domestic and international interests in recent years. Originated from $(C_4\ H_9O)_4Ti$,nano-rutile TiO_2 was synthesized by low temperature hydrolytic process in this paper.After being prepared by decomposing ammonium tungstate and covering on the surface of TiO_2, TiO_2/WO_3 were characterized by means of thermogravimetric and differential scanning calorimeter (TG-DSC), X-ray diffratction (XRD), UV-vis diffuse reflectance (DRS), fluorescence spectrum (FS). Results showed that with the increase of the supported concentration of WO_3 the reflectance of DRS and the fluorescence spectrum intensity of TiO_2/WO_3 decreased accordingly which indicated the powder's increase in light absorbance and the decrease in luminescence respectively.

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Vibration Damping of High-Chromium Ferromagnetic Steel: *Satish Bhujang Mutt*[1]; Mahesh Kumbeshwara[1]; Girish Bhujang Mutt[1]; [1]East Point College of Engineering and Technology

The present work aims to study the effect of annealing on the vibration damping capacity of high-chromium (16%) ferromagnetic steel. The alloys were prepared from raw materials of 99.9% purity melted in a high frequency induction furnace under vacuum. The samples were heat-treated in vacuum temperatures (800 to 1200ºC) for 1 hour followed by slow cooling (120ºC/h). The inverted torsional pendulum method was used to evaluate the vibration damping capacity. A water-based magneto-fluid was used to analyze magnetic domain morphology of the alloy using optical microscopy. The results indicated that the vibration damping capacity of the alloys is influenced by annealing and there exists a critical annealing temperature after 1000ºC. The damping capacity increases quickly below the critical temperature since the magnetic domains move more easily. Above the critical temperature the damping capacity decreases due to the larger size of the magnetic domains leading to decrease in domain wall area.

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Corrosion Mechanism of A3 Steel Induced by Chloride Ions in the Purified Water: Liyuan Chai[1]; Haijuan Xiao[1]; *Yunyan Wang*[1]; Yude Shu[1]; Fei Pei[1]; Jinlong Zhang[1]; [1]Central South University

In the nonferrous metallurgical industry it is of great significance to solve the problem of resource waste and environment pollution due to the discharge of heavy metal-containing wastewater. However, there arises a question whether the water impurities with chloride ions and fluoride ions will result in the corrosion of the pipeline during the whole recycling process. In this study, the corrosion mechanism of A3 steel induced by chloride ions in the purified water had been investigated with the A C Impedance technique. The results showed that there were another two factors which determined its electrochemical corrosive rate: the electrode potential and coverage ratio of chloride ions on the surface of A3 Steel. The corrosion mechanism of A3 steel in the solution with chloride ions emendation was two steps of electrode process with the rate-determining step of FeCl Fe2+ +Cl- +e-.

Computational Thermodynamics and Kinetics: Thin Films

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

Monday PM — Room: 3002
February 16, 2009 — Location: Moscone West Convention Center

Session Chair: Pascal Bellon, University of Illinois

2:00 PM Introductory Comments

2:05 PM Invited
Stress-Driven Surface Evolution during Whisker and Hillock Formation: *W. J. Boettinger*[1]; T. Frolov[2]; V. A. Ivanov[2]; Y. Mishin[2]; [1]National Institute of Standards and Technology; [2]George Mason University

In stressed solids, surface evolution is often driven by grain boundary diffusion and can result in growth of hillocks and whiskers. Examples are whisker growth in compressively stressed Sn deposits on Cu and hillock formation in Cu conductor lines during electromigration. The mechanisms of hillock and whisker growth remain largely unknown. We present molecular dynamics simulations aimed at understanding the conditions (stress, temperature, grain boundary diffusion, surface diffusion) at which the hillock/whisker growth processes can be initiated. The simulated geometries include a single boundary normal to the surface and a tri-crystal with a wedge-shape surface grain, both under an applied stress parallel to the surface. We have also studied extrusion of materials through a nano-hole simulating a crack in an oxide layer covering a stressed film. The early stage of hillock/whisker growth is observed at high homologous temperatures when the boundary diffusion flux exceeds the lateral fluxes of surface diffusion.

2:35 PM Invited
Effects of Substrate Symmetry and Prepatterning on the Stability of Compositional Patterns in Ultrathin Alloy Films: Bo Yang[1]; Tejodher Mupidi[1]; Vidvuds Ozolins[1]; *Mark Asta*[1]; [1]University of California

First-principles-based computer simulations are employed to elucidate the effects of substrate symmetry and externally applied prepatterned "potentials" on directing self-assembly of ordered nanoscale compositional patterns in ultrathin films. This work focuses on alloy films as a specific example where the energetics underlying composition modulation can be accurately quantified within the framework of a hybrid model that incorporates an atomistic calculation of interatomic bonding with continuum theories of long-range substrate-mediated elastic interactions. Employing Monte-Carlo simulations based on this hybrid model for alloy energetics, we demonstrate that even relatively weak external potentials, with periodicities considerably larger than the intrinsic composition-modulation wavelengths, can be highly effective in stabilizing ordered compositional patterns at the nanoscale.

3:05 PM
Compositional Domain Formation in Ultrathin Films: A Phase-Field Crystal Study: *Srevatsan Muralidharan*[1]; Mikko Haataja[1]; [1]Princeton Univ

It is well-known that materials confined in one or more dimensions may display properties which are strikingly different from those of their bulk counterparts. An illustrative example of this phenomenon is provided by a binary alloy, which is immiscible in the bulk and yet forms miscible phases when deposited on a surface as a (sub)monolayer aggregate. In this case, the mixing of the components is brought upon by the epitaxial nature of the growth processes. In addition to alloying, surface dislocations provide a mechanism for strain relaxation. In this talk we describe a phase-field crystal (PFC) model we have recently developed to study this technologically relevant process. The PFC model incorporates alloy thermodynamics, the presence and motion of free surfaces and/or grain boundaries, the presence of long-ranged elastic strains, and the nucleation and dynamics of dislocations, thus providing a physically-based picture of the domain formation kinetics at the nanoscale.

3:25 PM
Coarsening of 3D Thin Films under the Influence of Strong Surface Anisotropy, Elastic Stresses: *Peng Zhou*[1]; Steven Wise[2]; John Lowengrub[1]; [1]University of California Irvine; [2]University of Tennessee Knoxville

We develop a diffuse interface model to investigate the three dimensional coarsening in thin films. In this model, both strong surface anisotropy with Willmore regularization, elastic stresses and deposition are included. The governing equation for the phase field parameter is a sixth order Cahn-Hilliard Equation due to the presence of surface anisotropy and the Willmore regularization. The simulated system is assumed to be in mechanical equilibrium with misfit in the film generated by lattice mismatch in the substrate. Thus, the Cauchy-Navier equations are solved for elastic displacements which lead to the elastic energy. Both the Cahn-Hilliard equation and the Cauchy-Navier equations are solved with an non-stiff, adaptive nonlinear multigrid method. Simulation results of coarsening in three dimensions with different strengths of the surface anisotropy, misfit strain, and deposition rates will be shown. Comparison and analyses of these results will help to explain their influence on coarsening processes in thin films.

3:45 PM Break

4:10 PM
Sintering and Microstructure Evolution in Columnar Thermal Barrier Coatings: *Ramanathan Krishnamurthy*[1]; David Srolovitz[2]; [1]Caterpillar Inc; [2]Yeshiva University

Sintering of thermal barrier coatings changes their key properties, thus adversely impacting their reliability. We present a hierarchical modeling approach to study sintering-induced evolution of topcoat microstructure, wherein the sintering of individual topcoat column pairs is modeled using a thermodynamic principle, and column center-to-center approach rates calculated thence are incorporated into a discrete dynamics model of the temporal evolution of hundreds of columns. Surface, grain boundary and strain energy effects are naturally included in this framework. Varied late-time microstructures, with small clusters and random in-plane porosity, or with 50-100 columns-wide clusters separated by elongated inter-cluster channels,are observed, corresponding to small/large extents of contact among 'feathery' protrusions from columns. Statistical measures extracted from predicted microstructures reveal that cluster formation is strongly favored for large column densities and extents of the 'feathery' protrusions from columns. We compare predicted microstructures with recent experimental observations and discuss their import for thermal barrier coating processing/reliability.

4:30 PM
Characterizing Adsorption on Metallic Surfaces: Effect of Composition: *Baskar Ganapathysubramanian*[1]; Nicholas Zabaras[2]; [1]Iowa State University; [2]Cornell University

The enhancement of adsorption of (hydrogen) molecules on metallic surfaces is a key challenge for producing feasible fuel storage technologies. The chemistry of the surface under consideration plays an essential part in the adsorption phenomena. A reliable computational framework requires very accurate first-principle calculations of the energy of the system. We utilize the recently developed weighted multi-body expansion to accurately represent the energy of a cluster of atoms. An adaptive sparse grid collocation strategy provides the ability to effectively tessellate high dimensional surfaces. This allows us to naturally incorporate higher order interactions (up to 5 body terms). We utilize this strategy to construct multibody potentials representing the interaction of hydrogen with various transition metals. We investigate the effect of composition variation on the absorption coefficient.

4:50 PM
Thermodynamics of Nanoscale Binary Systems: *Muralidharan Ramachandran*[1]; Ramana Reddy[1]; [1]The University of Alabama

Nanoscale materials have been considered for and been in use in a variety of industrial engineering applications. It is shown that the melting temperature decreases and the phase diagram of binary systems change with the decrease in particle size. Non-ideal or real solution characteristics were introduced into the binary system using the activity data obtained from the literature. The phase diagrams of selected nanoscale binary systems were constructed considering the non-ideality of the system, the surface effects and the variation in the particle size and shape. The availability of data on surface and interfacial tensions has limited the number of systems considered. The calculated results were compared with that of the experimental results from the literature.

5:10 PM
Simulation of Thickness Effect on Grain Growth in Thin Films and Experimental Verification: Zhinan An[1]; *Yonghua Rong*[1]; [1]Shanghai Jiao Tong University

Various stagnation effects of grain growth in nano materials have been found, but thickness effect has not yet been researched. This paper presents an anisotropic Monte Carlo (MC) algorism to stimulate grain growth in thin films in annealing process. The simulation results reveal that thickness effect begins to work only when the average grain size reaches 0.8 to 1.2 times of the thickness of the film, not in the whole process of grain growth. Experimental data of grain growth in pure Co films with different thicknesses confirm the simulation results. Based on the stimulation and experiments, a modified grain growth kinetic equation is suggested to better describe the whole process of grain growth in nano-films.

5:30 PM
Effect of Partical Failure on the Yield Strength of SiCp/Al Matrix Composites: *Dai-hong Xiao*[1]; [1]Central South University

The SiC particles stress in aluminum matrix composites was examined according to the Eshelby's equivalent inclusion approach. A model was established to examine the influence of SiC particles failure on the yield strength of SiCp/Al composites after assumption that the SiC particles failure follows Weibull statistics. The values of tensile strength of SiCp/Al composites predicted by the model are well agreed with the experimental values. Moreover, the interface debond is the main failure way when the particle diameter is small in yielding condition, the percentage of particle fracture was found to increases with the increase of particles volume fraction and play the more important role in particle failure.