3:10 PM
Phase Stability and Transformations in NiTi from Density Functional Theory Calculations: *Karthik` Guda Vishnu*[1]; Alejandro Strachan[1]; [1]Purdue University

We used density functional theory to characterize various crystalline phases of NiTi alloys: i) high temperature austenite phase B2, ii) orthorhombic B19, iii) the monoclinic martensite phase B19', and iv) a body centered orthorhombic phase (B33), theoretically predicted to be the ground state. We also investigated possible transition pathways between the various phases and the energetics involved. Interestingly, We predict a new phase of NiTi, denoted B19", which is involved in the transition between B19' and BCO. B19" is monoclinic and can exhibit shape memory. We find B19 to be metastable with a 4 meV energy barrier separating it from B19'. We would also like to show our large scale molecular dynamics (MD) simulation results to understand the role of size in martensitic transformation at nano scale.

3:30 PM Break

3:50 PM Invited
Coupled Continuum - Density Functional Theory Investigation of Crack-Tip Propagation and Dislocation Nucleation: Arun Nair[1]; *Derek Warner*[1]; Richard Hennig[1]; [1]Cornell University

Atomic-scale modeling of deformation processes has long been plagued by the challenge of accurately and efficiently describing the complexities of multispecies bonding. In the case of metals, this has lead to the majority of the atomistic modeling effort focusing on pure elemental metals in a vacuum, rather than more technologically relevant problems involving alloys with impurities in realistic environments. In an attempt to address this long-standing challenge we have employed a concurrent multi-scale approach that couples an atomistic region whose forces are calculated via Kohn-Sham Density Functional Theory to a continuum region described by linear elasticity. This approach enables us to examine large simulation cell sizes and thus properly account for the long-range elastic fields associated with key defects such as dislocations. This talk will specifically focus on the application of the above method to crack-tip phenomenon in aluminum in the presence of oxygen.

4:20 PM
Modeling of Magnetic Thin Film with Misfit Dislocations: *Nirand Pisutha-Arnond*[1]; Bo Yang[2]; Dong-Hee Lim[1]; Mark Asta[2]; Katsuyo Thornton[1]; [1]University of Michigan; [2]University of California, Davis

We present multiscale calculations of misfit dislocations to study dislocation energetics and structures within heteroepitaxial Fe films grown on Mo(110) and W(110) substrates. On the atomic level, we calculate the generalized stacking fault energies of the Fe/Mo and Fe/W systems from the density functional thoery, which are used as an input to the continuum models. On the continuum level, the Peierls-Nabarro formulation is employed to calculate the elastic field originating from the misfit dislocations within a film of finite thickness. The semi-analytical and numerical methods are used for planar and non planar films. By allowing the dislocation spacing to vary and by including the effect of homogeneous strain, the equilibrium dislocation spacing as a function of film thickness is obtained. We relate these results to the surface instability mechanism and the metastable height observed in the Fe/Mo and Fe/W systems.

4:40 PM
Strain Engineering on Si/Ge Nanoscale Heterostructures: *Yumi Park*[1]; Winnie Tan[1]; Alejandro Strachan[1]; [1]Purdue University

Strained heterostructures are ubiquitous in microelectronic applications and the ability to control strain is critical to improve their electronic properties. We use molecular dynamics to explore nanopatterning and local amorphization followed by re-crystallization as possible avenues for strain engineering. Nanopatterning of strained Si/Ge/Si heterostructures into 1-D bars leads to transverse strain relaxation in the Ge section due to surface relaxation and we characterize how this relaxation increases with decreasing the bar width (W) and increasing the Ge thickness (H). Local amorphization of Si/Ge nanolamintes also leads to strain relaxation in the direction normal to the crystal/amorphous interface that increases as the height of Si/Ge bi-layer (H) increases and the periodic length of the crystalline/amorphous pattern (W) decreases. In both cases, a full strain relaxation is achieved for roughly square cross section (H≈W) leading to a uniaxial strain state, which is desirable for high-speed electronics.

5:00 PM
Anomalous Dissipation in Single-Walled Carbon Nanotube Resonators: *Peter Greaney*[1]; Giovanna Lani[2]; Giancarlo Cicero[3]; Jeffrey Grossman[1]; [1]Massachusetts Institute of Technology; [2]Ecole Polytechnique; [3]Polytechnic of Torino

We observe transient anomalous dissipation during molecular dynamics simulation of the ring-down of flexural modes in single-walled carbon nanotube (CNT) resonators. During the anomalous regime the quality factor of the mode can be reduced by more than 95% for tens of picoseconds. The anomalous dissipation is sensitive to the CNT temperature and the energy in the mode, and remarkably increasing the excitation energy in the resonator causes it to decay to zero faster. This counter intuitive phenomenon is analogous to the Mpemba effect in the freezing of water, and as with the Mpemba effect, it implies that the background temperature in the system does not uniquely define its dissipative state. Using a projection algorithm we are able to follow the energy as it dissipates, identifying gateway modes that mediate the dissipation, and a resulting athermal phonon population. The implications for these observations for continuously driven resonators are discussed.

Neutron and X-Ray Studies of Advanced Materials III: Diffuse Scattering II

Sponsored by: The Minerals, Metals and Materials Society, ASM International, TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee, TMS: Titanium Committee
Program Organizers: Rozaliya Barabash, Oak Ridge National Laboratory; Jaimie Tiley, Air Force Research Laboratory; Erica Lilleodden, GKSS Research Center; Peter Liaw, University of Tennessee; Yandong Wang, Northeastern University

Wednesday PM Room: 303
February 17, 2010 Location: Washington State Convention Center

Session Chairs: Darren Goosens, Australian national University; Yang Ren, Argonne National Laboratory

2:00 PM Keynote
Monte Carlo Simulation of Disorder in the Ag^+ Fast Ion Conductors Pearceite and Polybasite: *Richard Welberry*[1]; [1]Research School of Chemistry

The pearceite–polybasite group of minerals (i.e. pearceite, antimonpearceite, arsenpolybasite and polybasite), of general stoichiometry $[M^{I}_{6}T^{III}_{2}S_{7}][Ag^{I}_{9}Cu^{I}S_{4}]$ with M=Ag^+, Cu^+ and T=As^{3+}, Sb^{3+}, occur relatively commonly in nature. All have recently been shown to exhibit Ag^+ fast ion conduction at rather low temperatures (only slightly above or below room temperature). The average crystal structure determination of these materials shows the positions of the Ag^+ ions to be smeared out or delocalised within sheets in an ordered framework structure comprised of the remaining ions. At the same time, strong and highly structured diffuse scattering has been observed which contains diffuse peaks that are incommensurate with the diffraction peaks of the framework structure. In order to try to understand the origins of the fast ion conduction properties of these materials we have used Monte Carlo computer simulation of a model system to interpret and analyse this observed diffuse scattering.

2:30 PM Invited
Monte Carlo Modelling of Diffuse Scattering from Single Crystals: *Darren Goossens*[1]; Aidan Heerdegen[1]; [1]Australian National University

Diffuse scattering probes the local ordering in a crystal, whereas Bragg peaks are descriptive of the average long-range ordering. The population of local configurations can be explored by modelling the three-dimensional distribution of diffuse scattering. Local configurations are not constrained by the average crystallographic symmetry so one way of modelling diffuse scattering is by modelling a disordered (short-range ordered) structure and then calculating its diffuse scattering. The structure must contain enough unit cells to give a statistically valid model of the populations of local configurations, and so requirements for a program to model this ordering are very different from programs which model average crystal structures (used to fit the Bragg diffraction). The strategies used to tackle the problem and the way in which they are implemented will be discussed.

2:50 PM Invited

Phase Transition under High Pressure in Ionic Liquid Based Mixtures: *Hiroshi Abe*[1]; Yusuke Imai[1]; Takefumi Goto[1]; Takahiro Takekiyo[1]; Yukihir Yoshimura[1]; [1]National Defense Academy

Room temperature ionic liquids (RTILs) have been big subjects of an environmentally "green" chemistry. Recently, anomalous domain growth was observed in [DEME][BF_4]-H_2O mixtures.[1] The anomaly causes superstructure and volume contractions.[2] In this study, we investigate isotope effect in hydrogen/deuterium (H_2O, DHO and D_2O) using [DEME][BF_4]-water mixtures by the simultaneous measurements. Crystallization temperature decreases by isotope effect in deuterium of water. Nucleation process in the mixture is suppressed instead of little water concentrations (≅ 1 mol%). At the same time, anomalous domain growth, superstructure and volume contractions disappear accompanied by the isotope effect of water. [1] Y. Imai, H. Abe, T. Goto, Y. Yoshimura, S. Kushiyama and H. Matsumoto, J. Phys. Chem. B 112, 9841 (2008). [2] Y. Imai, H. Abe and Y. Yoshimura, J. Phys. Chem. B 113, 2013 (2009).

3:10 PM Invited

Synchrotron High-Energy X-Ray Study of Advanced Materials with Nano-Scale Structures: *Yang Ren*[1]; Valeri Petkov[2]; Yandong Wang[3]; Zhihua Nie[3]; Dongmei Liu[4]; Peter Liaw[5]; [1]Argonne National Laboratory; [2]Central Michigan University; [3]Beijing Institute of Technology; [4]Northeastern University; [5]University of Tennessee

Materials with nano-scale structures have a broad range of applications and detailed knowledge of their atomic-level structure is essential in order to understand and predict their properties and functionalities. Nano-scale structures include nano-particles, nanocrystalline metals and alloys, nano-size precipitates in bulk samples, nano-twins, defects and local disorders, etc. Synchrotron high-energy x-rays are widely used to study the structure, phase transformation and mechanical properties of nano-materials. Among them, a non-traditional approach based on high-energy x-ray total diffraction and atomic pair distribution function data analysis and structure simulations has been developed to investigate the atomic level structures of nanomaterials, that can be performed in various conditions, In this talk, we will present our recent work in this area, including the principle of the method, experimental facility and scientific results of different nanostructures. (Use of the Advanced Photon Source was supported by the U. S. DOE, Office of Science, under Contract No. DE-AC02-06CH11357.)

3:30 PM Invited

Unlocking the 'True' Structure of Complex Materials Using Total Scattering: *Thomas Proffen*[1]; [1]Los Alamos National Laboratory

Total scattering is becoming crucial tool to understanding the atomic structure of complex materials. Conventional structure determination based on Bragg scattering and yields the average structure of the material. However, many modern materials owe their properties to defects or their nano-crystalline character makes conventional Bragg analysis difficult or impossible. New neutron and X-ray instrumentation as well s advances in data reduction and modeling software are making total scattering analysis more accessible and add an invaluable characterization tool for complex materials. Recent developments as well as a cross section of recent applications of this technique will be discussed.

3:50 PM

X-Ray Diffraction Investigation of Ferroelectric Constitutive Behavior at Multiple Length Scales: Goknur Tutuncu[1]; Mesut Varlioglu[1]; Ulrich Lienert[2]; *Ersan Ustundag*[1]; [1]Iowa State University; [2]Argonne National Laboratory

The complex response of ferroelectrics to electromechanical loading requires rigorous characterization of their internal stresses and texture at multiple length scales to fully appreciate their constitutive behavior. *MACROSCALE*: Lattice strain and domain switching (texture) in polycrystalline BaTiO3 under electric field and/or mechanical loading were measured along multiple directions simultaneously. It was seen the lattice strain data are highly anisotropic resulting in large differences between hkl-specific strains. In addition, texture analysis suggests non-180° domain switching is tightly coupled with lattice strain evolution. *MESOSCALE*: The 3D-XRD X-ray diffraction technique was employed to probe the constitutive behavior of individual grains of polycrystalline BaTiO3 under electric field. In addition, domain variants of those grains were identified and their evolution was monitored as a function of applied field and temperature. 3-D XRD data correlate well with the macroscale results, but also yield valuable information about local variations at the mesoscale.

4:05 PM

Imaging Strains on the Nanoscale with Coherent X-Ray Diffraction Microscopy: *Ross Harder*[1]; Loren Beitra[2]; Steven Leake[2]; Marcus Newton[3]; Ian Robinson[2]; [1]Argonne National Lab; [2]University College London; [3]University of Surrey

Nanocrystals are being developed for a great range of applications. Strain on the nanometer scale within these structures has a great impact on their electronic properties. Coherent x-ray diffraction(CXD) microscopy done around the Bragg peaks of nanocrystalline samples have shown remarkable sensitivity to strain within the crystal structure. Recent improvements in CXD instrumentation at the Advanced Photon Source have allowed us to measure CXD patterns around multiple Bragg peaks of isolated nanocrystals of gold and zinc oxide. When each of these Bragg peaks is inverted to direct space the 3D image contains one projection of the distortion of the nanocrystal lattice within the crystal. These separate images have been combined into a fully three-dimensional image of the distortion field of the lattice of the nanocrystals. The full strain tensor of the material in 3D can then be visualized. Our imaging of the strain within nanocrystals will be discussed.

4:20 PM Break

4:30 PM Invited

Geometry, Topology and Structure of Amorphous Solids: *Zbigniew Stachurski*[1]; Richard Welberry[1]; [1]Australian National University

The understanding of the structure of solids began with the concept of translational symmetry, and has to a large degree come about because of the methods of X-ray crystallography. Frank and Kasper considered the topology of clusters of atoms instead of crystallographic unit cell. They distinguished three cases: (1) Coordination shell atoms make equilateral triangles with the centre. (2) Triangles in coordination shell are equilateral; shell atoms make isosceles triangles with the centre. (3) No requirements on the shape of the triangles within the shell. The third case provides a basis for development of a model of a completely random structure (ideal amorphous solid). A model of Zr-based metallic glass has been constructed and described. Debye x-ray scattering computations can reveal the presence of vacancies and other imperfections. Two new atomic mechanisms are identified as the fundamental means of compositional re-distribution in the alloy.

4:50 PM Invited

In-Situ Neutron Diffraction Study of B2 CoTi and CoZr: Rupalee Mulay[1]; James Wollmershauser[1]; *Sean Agnew*[1]; [1]University of Virginia

Fully-ordered B2 intermetallic compounds, CoTi and CoZr, are examined by in-situ neutron diffraction during compression testing. The results reiterate that the primary slip systems in these materials are <100> {011}, but also exposed a deformation mechanism transition that helps to explain the anomalous ductility of these compounds. Previous studies revealed kink banding, under some conditions. Preliminary cyclic tension tests carried out on these materials have shown that they exhibit a strong Bauschinger effect, and recent publications in the literature have emphasized a possible connection between "incipient kink banding" and such strong Bauschinger effects. However, preliminary polycrystal plasticity modeling predicts a similarly strong Bauschinger effect in CoZr without the incorporation of a kink banding mechanism, rather intergranular stresses create the effect. Cyclic in-situ neutron diffraction and electron back-scattered diffraction studies of CoTi and CoZr are being used to determine the role of kink banding in the deformation of these materials.

5:10 PM

Influence of Calcium and Strontium Substitution on the Expansion Behaviors and Oxygen Vacancy Concentration of the Lanthanum Ferrite: *David Thomsen*[1]; Patrick Price[1]; Ellen Rabenberg[1]; Darryl Butt[1]; [1]Boise State University

X-ray diffraction (XRD) was used to investigate the lattice expansion behavior of LaxCa1-xFeO3-d and LaxSr1-xFeO3-d which are mixed ion conductor. LaxCa1-xFeO3-d and LaxSr1-xFeO3-d samples were made by solid state method from 0 = x = 1. The Bruker AXS D8 Discover high-resolution XRD was used to measure the lattice as a function of temperature. XRD has the ability to isolate the lattice parameter with negligible effect from changing vacancy concentration. By comparison, dilatometry measures bulk thermal expansion,