SYMPOSIUM AA

Micro- and Nanomechanics of Structural Materials

November 28 - December 2, 2005

Chairs

William A. Curtin
Division of Engineering
Brown University
Box D
Providence, RI 02912
401-863-1418

Mark F. Horstemeyer
Dept. of Mechanical Engineering
Mississippi State University
MS 9552
P.O. Box ME
Mississippi State, MS 39762
662-325-7308

Alfonso H. Ngan
Dept. of Mechanical Engineering
University of Hong Kong
Haking Wong Bldg.
Pokfulam Rd.
Hong Kong, China
852-2859-7900

Louis Hector
General Motors R&D Center
MS 480-106-224
30500 Mound Rd.
Warren, MI 48090-9055
586-986-0587

Symposium Support
Alcoa Inc.
Northrop Grumman Corporation
Pratt & Whitney
Defense Advanced Research Projects Agency, Defense Sciences Office

* Invited paper

SESSION AA1: Ab-initio and Grain Boundaries
Chair: L. Hector
Monday Morning, November 28, 2005
Republic B (Sheraton)

8:00 AM AA1.1
Multiscale Simulations of High-Temperature Fracture in Silicon. Noam Bernstein, Center for Computational Materials Science, Naval Research Laboratory, Washington, District of Columbia.

While usually thought of as a functional material, silicon is used as a structural material in micro-electromechanical systems (MEMS), and it is also the model system for the brittle to ductile transition. Mechanics of nanoscale features, from crack tips to dislocation cores, control the failure of silicon by brittle fracture or by plastic deformation. I present simulations of dynamic fracture in silicon that combine a quantum-mechanical description of bonding near the crack tip with an empirical potential description of the rest of the loaded material. The dynamically coupled method [1] uses a tight-binding total energy model for silicon with a constrained real-space Green's function solution for the electron density, mechanically coupled to an empirical potential based on the Stillinger-Weber functional form. I apply this method to the propagation of a notch in a single crystal silicon sample at finite temperatures. At low temperatures the simulations show ideal brittle fracture, in agreement with experiment, with a velocity gap but minimal lattice trapping. At high temperatures fluctuations affect the crack propagation process and defects form spontaneously at the crack tip, although the velocity gap remains significant. These results show the effects of temperature on brittle fracture, and the atomic scale processes that lead to nucleation of dislocations above the brittle to ductile transition temperature. [1] N. Bernstein and D. Hess, MRS Proc. **653** (2001); – Phys. Rev. Lett. **91** (2003).

8:15 AM AA1.2
First Principles Studies of Screw and Edge Dislocation Cores in Pure Aluminum. Louis Gerard Hector[1], Chris Woodward[2], Dallas Trinkle[3], David Olmsted[4] and William Curtin[5]; [1]Materials and Processes Lab, GM R&D Center, Warren, Michigan; [2]Physics Dept., Ohio State University, Columbus, Ohio; [3]Materials Science Dept., Nortwestern University, Evanston, Illinois; [4]Division of Engineering, Brown University, Providence, Rhode Island; [5]Division of Engineering, Brown University, Providence, Rhode Island.

Aluminum screw and edge dislocation cores were optimized using a first principles approach together with a lattice Green's function.

8:30 AM *AA1.3
Hydrogen Embrittlement of Aluminum: First-Principles Calculations and Multiscale Simulations. Efthimios Kaxiras[1], Gang Lu[2] and Ellad Tadmor[3]; [1]Physics Department and Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts; [2]Department of Physics and Astronomy, California State Uiversity, Northridge, California; [3]Mechanical Engineering Department, Technion - Israel Institute of Technology, Haifa, Israel.

The effects of impurities in the embrittlement of metals are well documented by experiment, but a picture based on microscopic, atomic-scale models is not easy to construct. This is in part because of the local nature of chemical interactions between the impurity and its immediate neighbors of the host lattice, and the long-range effects that this local interaction produces. In order to address such issues, we chose aluminum as the prototypical ductile solid and hydrogen as an impurity which is ubiquitous and has been studied widely for its embrittling properties. We have performed first-principles electronic structure calculations to elucidate the interplay between hydrogen impurities and native defects in Al such as vacancies, as well as mutliscale simulations to investigate the effect of hydrogen impurities on dislocation properties. We will report some of the main conclusions emerging from these studies as well as on-going efforts to extend the accuracy and range of the theoretical methods.

9:00 AM AA1.4
Quanititative modeling of solid-solution softening in BCC Mo at the atomistic scale. Dallas Trinkle and Christopher Woodward; MLLMD, AFRL, Dayton, Ohio.

Solid solution softening observed in the group VA and group VIA transition metals has traditionally been attributed to either extrinsic–such as interstitial scavanging–or intrinsic–direct solute/dislocation interaction–effects. We model intrinsic mechanisms using first principles methods and accurately describe softening in Mo with 5d solutes. The prediction of strength with alloy concentration and temperature for Mo alloys requires two steps: (1) the calculation of the direct solute-dislocation interaction, and (2) the modeling of those effects on the motion of dislocations, and ultimately, plasticity. We calculate the interaction energy of a screw dislocation and a solute (Hf, Ta, Re, Os, Ir, and Pt) at the atomic level using state-of-the-art quantum-mechanical electronic structure methods. Furthermore, we compute the change in resistance to the motion of the dislocation in the presence of solutes. We incorporate our interaction data into a solid-solution softening model for the double-kink nucleation and kink-migration enthalpy barriers. The final model is able to quantitatively predict strength measurements of Mo-Re, and match hardness measurements of Mo-Pt: two systems with dramatically different softening and hardening behavior.

9:15 AM AA1.5
Intrinsic Strength, Elastic Property, and Electronic Structure of Ti-V BCC Alloys. Tianshu Li[1,2], John Williams Morris[1,2] and Daryl C. Chrzan[1,2]; [1]Department of Materials Science and Engineering, University of California at Berkeley, Berkeley, California; [2]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California.

Recently developed "gum metals" (multifunctional Ti-based superalloys*) exhibit many superior structural properties, *e.g.*, super elasticity, super plasticity, ultralow elastic modulus and ultrahigh strength. The experimentally observed dislocation-free plastic deformation mechanism raises the possibility that the ideal strength dominates the structural properties of these alloys. In this study, an examination of the ideal strength in Ti-V binary alloys is conducted using an *abinitio* electronic structure total energy method and the virtual crystal approximation. The calculations show low intrinsic strengths that are comparable with the experimental measurements when the electron to atom ratio approaches the specific value associated with "gum metals". The predicted elastic properties of alloys at different concentrations are also in good agreement with the experiment. The variations of the intrinsic strength and elastic proprieties are found to be correlated with both thermodynamical and dynamical stabilities of BCC, FCC and HCP structures. The study thus provides a theoretical basis for understanding the complex behaviors in "gum metals". This work is supported by Toyota Research and Development. *Takashi Saito, Tadahiko Furuta, Jung-Hwan Hwang, Shigeru Kuramoto, Kazuaki Nishino, Nobuaki Suzuki, Rong Chen, Akira Yamada, Yoshiki Seno, Takamasa Nonaka, et al., Science 300, 464 (2003).

9:30 AM AA1.6
First-principles calculations on the embrittlement mechanism of bcc iron grain boundaries by impurity segregation. Masatake Yamaguchi[1], Yutaka Nishiyama[2], Motoyuki Shiga[1] and Hideo Kaburaki[1]; [1]Center for Promotion of Computational Science and Engineering, Japan Atomic Energy Research Institute, Tokai, Ibaraki, Japan; [2]Department of Reactor Safety Research, Japan Atomic Energy Research Institute, Tokai, Ibaraki, Japan.

First-principles method is applied to assess the embrittlement mechanism of bcc iron (Fe) grain boundaries due to the segregation of sulfur (S) and phosphorus (P) impurities. It is a well-known experimental fact that the embrittlement of bcc iron occurs due to the segregation of S and/or P impurities to grain boundaries. However, its embrittlement mechanism is not clearly understood at the atomistic level. A simulation method based on the first-principles calculations has been proposed and applied to clarify this mechanism. This method consists of two stages. One is the detailed first-principles calculation of segregation energy for different configurations of impurity atoms near the grain boundary. The obtained energy for a particular configuration of impurities is compared with the statistical segregation model (McLean's equation) to evaluate whether the segregation is possible or not. The other is the tensile test simulation using the first-principles calculations where the total binding energy of the two crystal grains is assessed as a function of atomic displacement. This method is applied to the bcc Fe $\Sigma3(111)$ symmetrical tilt grain boundary to evaluate the effects of S and P segregation on the embrittlement. For the case of S segregation, we have found that the presence of a small amount of S atoms, nearly 20-30 ppm in the bulk, causes a strong embrittlement of a grain boundary, that is, the tensile strength reduces to one-tenth of that of a clean grain boundary due to the strong repulsion between sulfur atoms. This mechanism is found to be coincided with our recently found mechanism of nickel-sulfur (Ni-S) system [M. Yamaguchi et al., Science 307, 393(2005)]. For the P segregation, we have found that the energy for one-layer segregation is very large. However, its energy reduces for more than one-layer segregation and becomes almost zero for two-layer P configuration. Depending on the condition of segregation, the reduction of the grain boundary strength is within 10-20% of the clean grain boundary. These facts correspond to the experimental data that embrittlement potency of P is almost one order lower than that of S [J. Kameda et al., Surf. Interface Anal. 31,522(2001)]. More results on the effects of different types of grain boundaries and impurities will be reported in the presentation.

9:45 AM AA1.7
Comprehensive Model of Nanostructures Strength.
Hyun Woo Shim, L. G. Zhou and Hanchen Huang; Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, New York.

We report the mechanics of nanostructures, particularly their variable elastic constants (or moduli). Using a combination of molecular statics and density functional theory based ab initio calculations, we proposed a model which describe six major factors; (1) the bond loss, (2) the bond saturation (or electron redistribution), (3) the surface reconstruction, (4) atomic bond chain alignments on surface, (5) the surface stress, and (6) the thickness of the plate. The model is verified through the comparison of the results with the covalent system and the metals with face-center-cubic, body-centered-cubic, and hexagonal-closed-packed structures. This model can be largely used for the nanomechanical applications such as nano-resonators to predict the frequency change accurately. It is noticeable there are controllable factors with surface treatments, which give us a large flexibility to design the nanomechanical systems.

10:30 AM *AA1.8
Atomistic Simulations of Grain Boundary Disclination Structure and Evolution in FCC Metals. David McDowell[1,2], Douglas E. Spearot[1] and Mark A. Tschopp[2]; [1]GWW School of Mechanical Engineering, Georgia Tech, Atlanta, Georgia; [2]School of Materials Science & Engineering, Georgia Tech, Atlanta, Georgia.

The objective of this work is to use atomistic simulations to explore grain boundary structure and its implications for inelastic behavior of FCC bicrystals and nanocrystalline materials. Dislocations and disclinations are used to characterize the grain boundary structure and evolution in bicrystal and nanocrystalline configurations. In this research, molecular statics (energy minimization) and molecular dynamics are used with an embedded atom method potential for pure FCC Cu and Al. First, energy minimization is performed on bicrystal interface models to study the 0K structure in terms of disclination content in grain boundaries. After an appropriate equilibration procedure, molecular dynamics simulations are performed at finite temperature to investigate structural rearrangement of the interface associated with dislocation nucleation. It is found that the distorted geometry of the interface after the trailing partial dislocation has been emitted may be characterized in terms of disclination dipoles. In complementary work, nanocrystalline grain structures are generated using a novel microrotation algorithm whereby the initial configuration with high angle grain boundaries is evolved to a lower energy configuration by introducing small rotational perturbations to the grain orientations prior to energy minimization for each Monte Carlo step. This work investigates the grain boundary disclination structure and evolution in nanocrystalline materials as a function of the grain size. Additionally, we examine the role of dislocations, disclinations and free volume in the deformation of nc materials. Characterizing the grain boundary structure and evolution in terms of dislocations and disclinations facilitates the linkage of discrete simulation results to continuum models that incorporate defect densities of both dislocation and disclination character.

11:00 AM AA1.9
Computer generated nanocrystalline grain boundary structures and their plastic deformation properties.
Anders Froseth, Peter M. Derlet and Helena Van Swygenhoven; Paul Scherrer Institution, Villigen PSI, Switzerland.

Experiments have consistently revealed that the plastic deformation properties of bulk metallic nanocrystalline materials depend sensitively on grain boundary structure and the missorientation topology of the grains: the connectivity of certain classes of grain boundaries throughout the sample. These factors are believed to play a fundamental role in the nature of the plasticity in terms of inter-granular sliding and dislocation activity within the grains, where molecular dynamic simulations have revealed that depending on the particular missorientation (and also grain orientation), a grain boundary can act as both a source and sink of dislocations (Nat. Mat. 3 (2004) 399). We present a methodology in which we can construct atomic configurations representing tailor made grain boundary network structures for use in large scale molecular dynamics simulations allowing, for example, the construction of clusters of grains containing either low angle, CSL or symmetric/non-symmetric sigma boundaries (Acta. Mat., in press (2005)). How these special grain boundaries influence the deformation behaviour in terms of dislocation activity and grain boundary sliding will be discussed.

11:15 AM AA1.10
Modeling the Barrier Strength and Nucleation Stress of Interfaces. Peter M. Anderson[1] and Richard G. Hoagland[2]; [1]Materials Science and Engineering, Ohio State University, Columbus, Ohio; [2]Materials Science and Technology, Los Alamos National Laboratory, Los Alamos, New Mexico.

The interaction between a dislocation and grain boundary or interface underlies inherent strengthening processes in polycrystalline and multiphase materials. Such interaction may not only dictate barrier strengths to dislocation pile-ups, but also control the ability of grain boundaries and interfaces to serve as dislocation nucleation sites. Indeed, experimental observations suggest that this dual barrier/nucleation role becomes more important for nanostructured polycrystals and nanolayered composites. This paper outlines continuum analyses that enable characterization of the barriers to slip through an interface due to moduli mismatch and interface shear. In the former case a barrier derives from the change in line energy due to the difference in elastic moduli of the adjoining phases; in the latter, a shearable interface attracts the dislocation because of image forces and a decrease in line energy as it enters the interface. These two cases are distinguished via the capacity of interfaces/grain boundaries to slide or open to accommodate changing dislocation content.

11:30 AM AA1.11
Multiscale Modeling of Dislocation/Grain Boundary Interactions. Michael P. Dewald and William A. Curtin; Engineering, Brown University, Providence, Rhode Island.

Dislocation mobility and grain boundary migration contribute significantly to plasticity in metals, but little is understood as to how interactions between them influence plastic response. A multiscale computational method (CADD) is used to study the effects of dislocation pile-ups at grain boundaries on the overall deformation and mechanical response of materials. Pile-ups of lattice dislocations are generated in the continuum and are driven towards a grain boundary. The junction of the lattice dislocations with the grain boundary is surrounded by an atomistic domain. Transference or reflections of lattice dislocations or nucleation of grain boundary dislocations can be detected and converted to discrete continuum descriptions and allowed to travel away from the atomistic/junction region. Recent modifications to CADD include the use of anisotropic elasticity to describe discrete dislocations outside a given radius from the dislocation core and a template dislocation core solution that is used within this radius. This template solution captures the non-linearity of the dislocation core structure which allows for more accurate details when dislocations are near the atomistic/continuum interface region. Anisotropic elasticity captures more accurately the long range effects of dislocations with other dislocations as well as with the atomistic/continuum interface. The effects of grain boundary structure and geometry, dislocation structure, pile-up densities, and applied loading on the absorption, transmission, and damage initiation at the grain boundary are studied. Preliminary results indicate that for FCC Aluminum singular tilt <110> grain boundaries act as strong sinks for full screw dislocations and strong barriers for full 60 degree dislocations.

11:45 AM AA1.12
Continuum Modeling of the Deformation Mechanisms in Nanocrystalline Metals: Discrete Crystal Plasticity, Grain Boundary Migration, and Grain Boundary Sliding.
D. H. Warner and J. F. Molinari; Mechanical Engineering, Johns Hopkins University, Baltimore, Maryland.

The numerical modeling of nanocrystalline metals provides a unique challenge. Due to the length and time scales associated with the problem, modeling must take place at the interface between continuum and atomistic domains. Although atomistic modeling of these materials is primarily restricted by computational expense, continuum modeling is limited by the difficult selection of appropriate constitutive laws. Furthermore, continuum modeling at these length scales is complicated by the numerical complexities associated with discrete bursts of plasticity and an evolving microstructure. In this work, we address both the numeric and constitutive difficulties associated with using a continuum model to simulate nanocrystalline metals. By performing parallel finite element simulations, the collective deformation of many grains can be investigated. The effect of grain size distribution on strength and ductility in nanocrystalline metals is shown. Moreover, the recently exposed role of microstructural evolution as a deformation mechanism is included in simulations which account for grain boundary motion during deformation. The dependence of the stress-strain curve on the evolving microstructure is presented. In addition to the adaptive meshing techniques necessary to simulate microstructural evolution, a discrete crystal plasticity model is developed to more accurately capture deformation within nanometer sized grains. The difficulties associated with this kind of model are highlighted as well as the perspective for resolving them. Finally, grain boundary sliding was included in the model using constitutive properties obtained from a hierarchical multi-scale approach in the form of independent atomistic calculations (QC-method). The influence of grain boundary sliding on plastic strain localization is noted.

SESSION AA2: Atomistics
Chair: W. Curtin
Monday Afternoon, November 28, 2005
Republic B (Sheraton)

1:30 PM *AA2.1
Effect of Evolving Solute Structures on the Mechanical Behavior of Solid Solutions. Catalin Picu, Rensselaer Polytechnic Institute, Troy, New York.

An experimental and combined atomistic, mesoscale and continuum modeling program was developed to investigate the influence of evolving solute structures on the mechanical response of solid solutions. By solute structures we understand clusters located at and away from dislocations, and nanoscale precipitates composed of several solute atoms. We focus on the Al-5%Mg binary alloy, which we take as a model system. The rate sensitivity of this material decreases as the solute concentration increases. The current mechanisms proposed to explain this phenomenon are discussed in light of the new findings. Specifically, we study bulk and pipe diffusion to dislocation cores looking for the size and structure of stable clusters, and the characteristic time of their growth. The effect of such clusters on dislocation mobility is assessed. Several new effects that lead to negative rate sensitivity will be presented and discussed against previously proposed mechanisms. Findings from the nano and mesoscale models are built into a slip system-level constitutive model of plastic deformation. The predictions of the model are compared with experimental data on strain rate sensitivity.

2:00 PM AA2.2
Molecular Dynamics Study of Solute Strengthening in Al/Mg Alloys. David Olmsted[1], Louis G. Hector[2] and William Curtin[1]; [1]Brown University, Providence, Rhode Island; [2]General Motors Technical Center, Warren, Michigan.

The strengthening of Al by Mg solute atoms is investigated using molecular dynamics (MD) studies of single dislocations moving through a field of randomly placed solutes. The MD method permits explicit treatment of core effects, dislocation pinning and deceleration, and dislocation unpinning by thermal activation, all under an applied load. Choice of an appropriate MD simulation cell size is assessed using analytic concepts developed by Labusch. The interaction energy of a single Mg atom with straight edge and screw dislocations is computed and compared with continuum models. Using the single Mg energies, a one-dimensional energy landscape for the motion of a straight edge dislocation through a random field of Mg solutes is computed. The minima in this landscape match well with those found in the MD simulations at zero temperature. The stress to unpin a straight edge dislocation trapped in a local energy minimum generated by the solutes is then predicted semi-analytically, and good agreement is obtained with the MD results. At temperatures of 300K and 500K, the thermally-activated rate of unpinning vs. stress and temperature is calculated semi-analytically, and agreement with the full MD results is again obtained with the fitting of a single attempt frequency in a transition state model. The agreement of the semi-analytical models provides a basis for calculating yield stress vs. strain rate and temperature, resulting from statistical pinning, for the case of non-interacting dislocations on a single slip system, and for ongoing work on dynamic strain aging effects resulting from diffusion of Mg atoms around a pinned dislocation.

2:15 PM AA2.3
Molecular dynamics and quasi-two dimensional dislocation dynamics simulations on the irradiation-induced hardening mechanism of FCC metals. Mitsuhiro Itakura[1], Tomoko Kadoyoshi[1], Hideo Kaburaki[1] and Shiro Jitsukawa[2]; [1]Center for Promotion of Computational Science and Engineering, Japan Atomic Energy Research Institute, Tokai, Ibaraki, Japan; [2]Department of Materials Science, Japan Atomic Energy Research Institute, Tokai, Ibaraki, Japan.

Molecular dynamics and quasi-two dimensional dislocation dynamics simulations have been performed to find the hardening mechanism of FCC metals due to irradiation. The focus of this simulation has been placed on the effects of the dissociation of a dislocation in FCC metals and of density, distribution, and strength of pinning centers on the stress-strain relation. Molecular dynamics method is applied to find the behavior of the interaction of an edge or a screw dislocation with a pinning center, such as a rigid sphere or irradiation-induced hexagonal interstitial cluster, and to measure its pinning strength by deriving the stress-strain relation. Copper (Cu) and aluminum (Al) EAM potentials have been used for the simulation to study the effects of dissociation width of a dislocation. For a hard sphere particle, the condition of the Orowan mechanism for bypassing a particle of various widths is determined with respect to the dissociation width of a dislocation. Also, we have found the condition of cross-slip for a screw dislocation encountering with a hard sphere particle. Molecular dynamics simulation is also performed for an interaction of a dislocation with an interstitial hexagonal cluster to study what kind of jog is formed and to determine its unpinning strength by the local stress-strain relation. These local pinning data are input to the dislocation dynamics simulation to study the global hardening characteristics. We have developed a quasi-two dimensional dislocation dynamics method by incorporating the effect of dissociation of a dislocation. The motion for a pair of dissociated partial dislocations is realized by introducing the binding stacking fault energy in the dislocation dynamics. This is verified for the interaction of a dissociated edge dislocation with a large interstitial cluster placed just below the slip plane by comparing with the molecular dynamics result. Since the width of an interstitial cluster is large compared with the dissociation width, the interaction between a dislocation and a cluster is elastic. The results of dislocation dynamics and molecular dynamics are found to be almost the same. With this quasi-two dimensional dislocation dynamics code, a new hardening stress-strain relation is obtained with particular emphasis on a high density distribution of pinning centers. The results for a relation of hardening and the dissociated width and shape of a dislocation are reported in the presentation.

3:30 PM AA2.4
Peierls Barrier for the Glide of 1/2<111> Screw Dislocations in BCC Metals Deduced from 0 K Atomistic Calculations and its Dependence on Non-Glide Stresses. Roman Groger and Vaclav Vitek; Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania.

Plastic flow of all bcc metals is controlled by a/2<111> screw dislocations that possess a high Peierls stress owing to their non-planar cores. At finite temperatures the corresponding Peierls barrier is surmounted via the formation of pairs of kinks. The crucial information for the development of the complete theory of the thermally activated motion of screw dislocations is the height and shape of the Peierls barrier together with its intrinsic dependence on the applied stress tensor. This information is not obtainable from any experimental data. Common atomistic studies at 0 K determine the Peierls stress and its dependence on the applied stress tensor but not directly the Peierls barrier. In this presentation, we will show that the shape of the Peierls barrier in bcc metals and its dependence on the loading can be extracted from the data obtained in atomistic studies at 0 K, specifically from the variation of the Peierls stress with the applied shear stresses parallel and perpendicular to the slip direction. For this purpose we consider the Peierls barrier as a two-dimensional periodic function of the position in the {111} plane. The effect of both the shear stress parallel and perpendicular to the slip direction enters via two adjustable terms the functional forms of which are based on the effective yield criterion recently developed for molybdenum on the basis of atomistic modeling of the screw dislocation and its glide at 0 K. The minimum energy path between two potential minima, and thus the corresponding activation barrier, was obtained using the Nudged Elastic Band method. The constructed Peierls barrier reproduces correctly not only the twinning-antitwinning asymmetry of the critical resolved shear stress for pure shear parallel to the slip direction but also the effect of shear stresses perpendicular to the slip direction. For molybdenum single crystals with all possible slip systems the yield surface predicted from the constructed Peierls potential agrees well with that calculated using the above-mentioned effective yield criterion. However, knowledge of the Peierls barrier, together with a model for the formation of the pairs of kinks, allows us to introduce the temperature and strain rate effects into the yield criteria. This advancement introduces for the first time the effect of both shear stresses parallel and perpendicular to the slip direction into the model of thermally activated dislocation motion. The effect of the latter stresses may be a significant decrease of the activation barrier for slip on the {110} planes with relatively small Schmid factors which may give rise to the "anomalous" slip often observed at low temperatures in pure bcc metals. This research was supported by the NSF Grant no. DMR02-19243.

3:45 PM AA2.5
The Dynamics of Glide of Screw Dislocations in BCC Fe: A Molecular Dynamics Approach. David Rodney, Julien Chaussidon and Marc Fivel; ENS de Physique, INP Grenoble, Saint Martin d'Heres, France.

The thermally-activated motion of the screw dislocations in BCC metals is one of the great challenges posed to both atomic and mesoscopic simulations. We are interested in a-iron. In this case, there are unknowns already at the level of the dislocation core: is it degenerated as predicted by pair potentials, or non-degenerated as obtained by recent ab-initio calculations? What about the role of non-Schmid effects such as the influence of non-glide stress

components? Also, why in atomic-scale simulations do screw dislocations glide on {112} planes, while experimentally, {110} glide planes are often observed? Finally, what is the dynamics of the double-kinks that can be in 2 {110} planes along a same line, giving rise to cross-kinks and debris left behind the dislocation. In order to clarify these points, we have undertaken a large program of atomic-scale Molecular Dynamics simulations of the glide of long screw dislocations at finite temperature. We investigate different stresses, different temperatures and compute directly from the simulations, as a function of these parameters, the average velocity of the screw dislocations, the nucleation rate of the double-kinks as well as their dynamics of expansion. We employ the Embedded Atom Method potential recently developed by Mendelev which predicts a non-degenerated core structure, in agreement with ab-initio calculations. Our aim is, in a multiscale approach, to extract the information required to construct a Dislocation Dynamics code that will account for the specificities of plasticity in BCC metals, which is not the case in any of the existing DD codes.

4:00 PM AA2.6
Atomistic Activation Energies for Homogeneous Dislocation Loop Nucleation. Robert D. Boyer[1] and Sidney Yip[2,1]; [1]Department of Materials Science and Engineering, MIT, Cambridge, Massachusetts; [2]Department of Nuclear Science and Engineering, MIT, Cambridge, Massachusetts.

Homogeneous dislocation loop nucleation is a fundamental problem in crystal plasticity that has been investigated extensively using both experimentation and continuum theories. We have applied the Nudged Elastic Band technique, along with empirical potentials of the Embedded Atom Method form, in an atomistic study of homogeneous dislocation loop nucleation in Cu perfect crystals. The potential, developed by Mishin et al, has been shown in previous work to quantitatively reproduce the atomistic relaxation mechanisms observed in ab initio calculations of homogeneous shear deformation. Here the activation barrier to dislocation nucleation and the atomistic features of the saddle point configuration will be presented for a range of shear stresses up to the critical stress at which a dislocation nucleates spontaneously. The effects of considering the full set of atomic degrees of freedom will be detailed in light of continuum studies already present in the literature with the goal of providing atomistic calibration for Peierls-Rice theories. Furthermore, implications of the entire reaction pathway from the onset of shear localization to the formation of an extended stacking fault will be discussed. This more fundamental study sheds light on previous work concerning dislocation nucleation at crack tips and will be used as a basis for continuing exploration of activation barriers for mechanisms of plastic deformation near pre-existing defects.

4:15 PM AA2.7
Molecular Dynamic Simulations of Hydrogen-Assisted Dislocation Nucleation and Nanovoid Nucleation. Mei Qiang[1], Mark Horstemeyer[1], Philip Gullett[2], Gregory Wagner[3] and Mike Baskes[4]; [1]Mechanical Engineering, Mississippi State University, Mississippi State, Mississippi; [2]Civil Engineering, Mississippi State University, Mississippi State, Mississippi; [3]Sandia National Laboratories, Livemore, California; [4]Materials Science & Technology Division, Los Alamos National Laboratories, Los Alamos, New Mexico.

We perform molecular dynamic simulations to study hydrogen-assisted dislocation nucleation and void nucleation at the atomic scale. Under straining, partial dislocations and deformation twins form in nickel lattice, and a void nucleates at one of the twin boundaries. Hydrogen interstitials appear to not affect dislocation nucleation and evolution, but cause void nucleation to occur at a lower applied stress and strain in nickel lattice. Under straining, dislocation tangles and sequential dislocation cell structures are formed in aluminum lattice. A void nucleates at an intersection of dislocation walls. Hydrogen interstitials cause dislocation nucleation and void nucleation to occur at a lower applied strain in aluminum lattice. They also appear to encourage dislocation tangles and cell structure formation in aluminum lattice. The percentage reduction of the strain for void nucleation and the strain for dislocation nucleation in aluminum lattice due to hydrogen interstitials is much higher than in nickel lattice. The simulation results suggest the hydrogen-assisted dislocation nucleation and void nucleation are strongly dependent on materials and the hydrogen concentrations.

4:30 PM AA2.8
Multiscale Modeling of Crack Tip Dislocation Emission and Hydrogen Embrittlement in BCC Iron. Shaoxing Qu and William A. Curtin; Engineering, Brown University, Providence, Rhode Island.

We have developed a finite-temperature dynamic coupled atomistic/discrete dislocation method which can be used to study thermal activation effect on the crystalline material properties. A thermostatting approach is applied to the motion of the atoms in a stadium region near the atom/continuum interface, while standard molecular dynamics algorithm is used in the interior region. FEM is adopted in the continuum region updated over time scales comparable to the Debye frequency. This approach, as well as Nose-Hoover thermostat, can achieve canonical-ensemble averages. The new multiscale modeling method has been used to study the behavior of ductile fracture in FCC aluminum with finite thickness along the crack front direction at finite temperature. In this paper, mode I fracture ({110}-type crack plane and <110>-type crack front) in BCC iron is studied using this new method with an EAM potential. It is shown that dislocation along two slip planes of the {112} type are available, which agrees with the observation from atomistic simulations. The hydrogen embrittlement effect on BCC iron is also investigated and the results are compared with those obtained from fully atomistic simulations.

4:45 PM AA2.9
Analytical and Simulation Studies of Crack Tip Plasticity. Sergio Picozzi[2] and Robin L. B. Selinger[1,2]; [1]Chemical Physics, Kent State University, Kent, Ohio; [2]Physics, Catholic University, Washington, District of Columbia.

The mechanical response of a sharp crack in a ductile solid depends on both the temperature and the stress state of the crack tip. At finite temperature, a crack under a subcritical applied load can emit dislocations via thermal activation, a process associated with creep. To estimate the relevant energy barrier and its dependence on applied stress, we use conformal mapping techniques in 2-d to solve a classical continuum elastostatics problem: a straight screw dislocation interacting with a sharp crack in a semi-infinite strip, loaded in mode III. We consider the hypothesis that the rate-limiting step in crack-tip plastic reponse is not dislocation nucleation but the escape of a fully formed dislocation from the attractive potential well surrounding the crack tip. We calculate that energy barrier and find that it drops exponentially as a function of increasing load. This result is compared with 2-d molecular dynamics simulation studies of ductile yield at a crack tip using an idealized potential. Simulation results demonstrate that the strain rate vs temperature follows Arrhenius behavior. Simulation results also confirm that the activation energy is a sensitive function of applied load.

SESSION AA3: Microstructure and Deformation
Chair: M. Horstemeyer
Tuesday Morning, November 29, 2005
Republic B (Sheraton)

8:00 AM *AA3.1
Computer Simulations of Realistic Microstructures of Discontinuously Reinforced Al-Alloy Composites and 7075 T6 Al-Alloy. Arun Gokhale, Harpreet Singh, Yuxiong Mao and Joel Harris; School of Materials Science & Engineering, Georgia Institute of Technology, Atlanta, Georgia.

Current methodologies for microstructure simulations mostly involve idealized simple particle/feature shapes, uniform-random spatial distribution of microstructural features, and isotropic feature orientations. However, the corresponding "real" microstructures often have complex feature shapes/morphologies, non-random/non-uniform spatial distributions, and partially anisotropic feature orientations. Consequently, such simulations do not capture these aspects of microstructural reality. In this contribution, we present a methodology that enables simulations of "realistic" microstructures where feature shapes/morphologies, spatial arrangement, and feature orientations are statistically similar to those in the corresponding real microstructures. The methodology is applied for simulations of microstructures of discontinuously reinforced aluminum (DRA) matrix composites and 7075 T6 Al-alloy. A small set of simulation parameters are used for generation of these microstructures, which are then correlated to the process parameters. These correlations permit generation of a set of virtual microstructures that cover a wide range of process conditions.

8:30 AM AA3.2
Computer Simulations of Realistic Microstructures of Ti-TiB Materials. Scott I. Lieberman[1], Yuxiong Mao[1], Arun M. Gokhale[1] and Seshacharyulu Tamirisakandala[2]; [1]School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia; [2]Department of Mechanical Engineering, Ohio University, Athens, Ohio.

A novel digital image processing based methodology has been implemented for simulating "realistic" material microstructures of Ti-TiB materials. The large variety of available processing methods and compositions of Ti-TiB materials, and the divergent performance

requirements for emerging aerospace and automotive applications, has increased the need for an efficient materials design capability. For useful quantitative prediction of the mechanical and physical properties of complex, real Ti-TiB microstructures, the methodology (1) incorporates realistic, complex particle/feature morphologies; (2) admits controlled non-uniformities in the spatial distributions of features; (3) permits partial anisotropic morphological orientations of microstructural features; (4) closely matches experimentally measured attributes of the corresponding real microstructures; and (5) can efficiently generate sufficiently large segments of microstructure that contain short, intermediate, and long range microstructural heterogeneities and spatial patterns. The microstructural simulation parameters can be correlated to the material processing conditions, and then used to generate a library of rational "virtual" microstructures to mimic the set of microstructures that would be created over a complete range of feasible process conditions. The virtual microstructures can then be implemented into computational models for materials properties and behavior, and correlations between the simulation parameters and the process conditions can be used to design and develop a material with the required microstructure that has the desired combination of properties.

8:45 AM *AA3.3
3D Digital Microstructures. Anthony Rollett[1], David Saylor[2], Joseph Fridy[3], Abhijit Brahme[1], Sukbin Lee[1], Stephen Sintay[1] and Robert Campman[1]; [1]Materials Sci. & Eng., Carnegie Mellon University, Pittsburgh, Pennsylvania; [2]CDRH-OSEL-DCMS, Food & Drug Administration, Rockville, Maryland; [3]Alcoa Technical Center, Pittsburgh, Pennsylvania.

A set of tools is described for creating digital three-dimensional microstructures based on statistical information from experimental measurements using automated electron back-scatter diffraction on orthogonal cross-sections. The microstructures currently allow grain shape, texture and grain boundary character to be matched to the measurements in a single-phase material. Grain shapes are abstracted in terms of distributions of either ellipsoids in 3D or ellipses in 2D sections. Grain orientation and grain boundary misorientation textures are quantified with distributions in a homochoric space. Simulated annealing is used to match the digital microstructures to the experimental information. The discretization of the microstructure can be realized by either a Voronoi tessellation or on a regular grid (voxels on a simple cubic lattice). Extensions of the method are described that generate finite element meshes based on either the tessellations or the regular grid. The resulting 3D digital microstructures are useful for a wide variety of applications. As an example, the kinetics and microstructural evolution, including texture, in a commercial purity aluminum have been modeled using this input. The results have shed new light on which factors are most significant in this vital aspect of metals processing.

9:15 AM AA3.4
Submicron-Resolution 3D X-Ray Structural Microscopy Characterization of Deformation Microstructure. Ben Larson[1], Wenge Yang[1,2] and Jon Tischler[1]; [1]Condensed Matter Sciences, Oak Ridge Nat. Lab., Oak Ridge, Tennessee; [2]Materials Science, Univ. of TN, Knoxville, Tennessee.

High-brilliance synchrotron x-ray sources and high-precision x-ray focusing optics have led to revolutionary advances in x-ray microscopy for the investigation of materials microstructure on mesoscopic length scales of tenths-of-microns to hundreds-of-microns. Differential-aperture x-ray structural microscopy (DAXM) using microbeams provides submicron-resolution 3D measurements of local crystal structure, orientation, and strain tensors in single-crystal, polycrystalline, and deformed materials. This measurement capability provides a direct and quantitative link between the actual microstructure and evolution in materials on mesoscopic length scales and the results of theory, simulation, and modeling. Micron resolution 3D measurements of the deformation microstructure generated by nano- and micro-indents in single crystal Cu made on the UNICAT-II beamline at the Advanced Photon Source will be discussed. Well developed lattice rotation and geometrically necessary dislocation (GND) density patterns observed tens of microns below indentations in <111> oriented Cu will be presented. The absolute, quantitative connection possible betweeen 3D x-ray microscopy measurements and detailed computer simulations and multi-scaled modeling will be discussed and opportunities for studies of fatigue and fracture will be considered. Research supported by the DOE Office of Science, Division of Materials Sciences under contract with ORNL, managed by UT-Battelle, LLC; UNI-CAT is supported by UIUC, ORNL, NIST and UOP Res., Inc. The APS is supported by the US Department of Energy.

10:00 AM *AA3.5
Application of Microstructure-Level Simulation to Life Cycle of Steel Components. Leo Chuzhoy[1], Clyde L. Briant[2], Alan Needleman[2] and Gerard M. Ludtka[3]; [1]Advanced Materials Technology, Caterpillar Inc., Peoria, Illinois; [2]Division of Engineering, Brown University, Providence, Rhode Island; [3]Metals & Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Steel is widely used for critical machine components in the heavy equipment industry. Microstructural elements such as grain size, inclusion and precipitate distributions, and chemistry control the performance of steel parts. Variation in these microstructural elements leads to variation in such critical properties as fatigue life, toughness, and wear resistance. Therefore, understanding and developing the ability to control the formation of steel microstructures and predicting its functional and environmental performance is critical to moving the industry closer to its energy efficiency, resource efficiency, and pollution prevention goals. The full realization of these benefits requires simulation tools that optimize the microstructure with respect to the mechanical and environmental performance throughout the life cycle of a particular steel component.

10:30 AM AA3.6
Damage and Crack Initiation Behaviour of Duplex Stainless Steel During Cyclic Loading. Guocai Chai[1] and Robert Lillbacka[2]; [1]Mechanical Metallurgy, Sandvik Materials Technology, Sandviken, Sweden; [2]Department of Applied Mechanics, Chalmers University of Technology, Goteborg, Sweden.

Duplex stainless steels are a group of stainless steels with a microstructure consisting of approximately equal volume of austenite and ferrite. Because of the respective physical and mechanical properties of each individual phase, these materials can suffer from non-uniform load sharing between the phases or stress heterogeneity on the microscopic scale, elastic/plastic anisotropy and other mechanical interactions on the scale of grain size during mechanical loading. In this work, the damage and crack initiation behaviour of a super duplex stainless steel during cyclic loading has been studied by both micro structural investigation and simulation using multiscale material modelling. Two material conditions, the anneal/quenched condition where the ferrite phase is slightly stronger than the austenite phase and the aged condition where the ferrite phase is much stronger than the austenite phase. It was found that the material damage and crack initiation start in the ferrite phase in the material with the anneal/quenched condition and in the either ferrite or austenite phase in the material with the aged condition, mainly in the weakest phase if the deformation hardening is considered. Simulation is generated using a Voronoi polygonization algorithm to model the grain structure, which results in a representative volume element (RVE). The crystallographic nature of the grains is modelled by crystal plasticity, and damage is introduced along the slip-systems of the crystal plasticity model. It shows how damage grows inside the grains and the crack initiation phase in duplex stainless steels during cyclic loading, which are comparable to the experimental observations.

10:45 AM AA3.7
Deformation and Failure Behavior of Resistance Spot Welded Dual Phase Steel. Hong Tao[1], Wei Tong[1], Louis G. Hector[2] and Pablo Zavattieri[2]; [1]Mechanical Engineering, Yale University, New Haven, Connecticut; [2]Research and Development Center, General Motors, Warren, Michigan.

As dual phase steel becomes a prospective automobile material due to its excellent combination of high strength and good ductility, the performance of resistance spot welded dual phase steel is currently under active evaluation. In this investigation, the deformation and failure behavior of resistance spot welded dual phase steel were characterized experimentally with the digital image correlation based strain mapping measurements. The tensile deformation and fracture behavior of the spot welded joints were simulated with the extracted material models of base, heat-affected and fusion material zones and two optimized micromechanics-based failure models.The optimized deformation model and failure models were then validated with the V-notched resistance spot welded dual phase steel plate sample.

11:00 AM AA3.8
Micromechanics Based Modelling of the Low and High Temperature Ductility of Aluminium Alloys. Denis Lassance, Damien Fabregue, Francis Delannay and Thomas Pardoen; Departement des Sciences des Materiaux et des Procedes, Universite Catholique de Louvain, Louvain-la-Neuve, Belgium.

The nucleation, growth and coalescence of voids in 6XXX Al alloys is investigated in order to captures the links between damage evolution, microstructure, temperature and extrusion conditions. The microstructure involves β-type elongated intermetallic particles, α-type rounded intermetallic particles, small disperoids and very small hardening precipitates. The relative proportion of α and β particles is varied by modifying the homogenization conditions. In-situ tensile testing within the SEM reveals that, at low temperature, the α

particles and the β particles oriented with the long axis perpendicular to the main loading direction undergo interface decohesion, while the β particle oriented with the main axis perpendicular to the main loading direction undergo fragmentation. At high temperatures, only interface decohesion is observed. Uniaxial tensile tests on notched and un-notched bars were performed for the different microstructures, at different temperatures ranging between 20C and 600C, at different loading rates and with different notch radii. The ductility increases with decreasing amount of β particles, increasing temperature, though with a drop around 580C, and decreasing stress triaxiality. An extended Gurson model has been developed in order to account for the complex hierarchy of damage mechanisms. The void nucleation law is a micro-macro model based on two critical stresses, one for interface decohesion and one for particle fracture. The critical stresses are assumed to be temperature independent. The voids resulting from particle decohesion, either from α or β particles, constitute the first population while the voids resulting from particle cracking are considered as a second population. If the temperature is larger than the melting temperature of the particles, voids are then assumed to be present from the beginning. The growth of the first population is estimated using a viscoplastic extension of the Gurson model accounting also for non-spherical void shapes. The void coalescence criterion assumes an internal necking process and takes into account the presence of the second population of voids which significantly decreases the strain at the onset of coalescence. The volume fractions and shapes of particles are measured experimentally. The temperature and rate dependent flow properties of the matrix material have been obtained by inverse modelling from the uniaxial tensile tests. The two critical stresses for the two void nucleation mechanisms are identified based on two different tests performed at two different temperatures on a microstructure involving both $\alpha$and β particles. The model is successfully validated by comparing the predictions with the large set of experimental data involving different relative proportion of α and β particles, temperatures and stress triaxialities.

11:15 AM AA3.9
Modeling and Testing of Magnesium Alloys with Temperature Dependence on Damage Evolution. Andrew Oppedal[1], Mark F. Horstemeyer[1], David L. Oglesby[1], Haitham El Kadiri[1] and Arun M. Gokhale[2]; [1]Center for Advanced Vehicular Systems, Mississippi State University, Mississippi State, Mississippi; [2]Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia.

Magnesium alloys such as AM50, AS21 and AE44 are becoming more prevalent in automotive applications ranging from steering wheels, dash components to front cross-members. Though the material is becoming more widely utilized, the temperature dependence on the damage evolution is still not well understood. The evolution of damage in a ductile material is known to comprise three mechanisms: void nucleation, growth, and coalescence. Each of these failure mechanisms has a different dependence on temperature. In this paper, we examine the temperature effects on void nucleation, growth and coalescence in several Mg alloys. We perform monotonic testing at several strain rates over a wide range of temperatures and quantify by post-mortem stereological analyses the pore fraction and size evolution using OM and SEM techniques. The fracture surfaces will be examined using SEM and surface topology measurement technique (via Talysurf). Finite element simulations are performed to compare with experimental results. Results of the testing will allow for more accurate modeling via finite element simulations of the material in predicting failure for product lifecycle conditions allowing for more optimal part design.

11:30 AM AA3.10
Modeling Dynamic Void Growth and Coalescence by Plasticity and Diffusion Using a Level Set Approach. Kinjal Dhruva[1], Alberto Cuitino[1] and Michael Ortiz[2]; [1]Mechanical & Aerospace Engineering, Rutgers University, Edison, New Jersey; [2]Graduate Aeronautical Laboratories, California Institute of Technology, Pasadena, California.

The study of dynamic failure of ductile material is particularly important in applications involving high impact loading characterized by high strain rates. Tensile waves are generated inside material at such high strain rates causing spall damage. As a result of spallation, voids are nucleated that subsequently grow until they merge together and coalesce forming microscopic cracks that eventually develop into fracture surface. We study the evolution of voids using a multi-scale approach in which the numerical model employs microscopic material properties to predict failure at a continuum level. The numerical scheme follows a unique approach of modeling void growth due to the combined effect of applied stress field and vacancy diffusion. It is achieved by using a Eulerian description of fields along with a level set description of void interface over a regular finite difference grid. This approach allows us to track complex topological changes in a natural way without any need of remeshing. The level set evolves under a non-uniform velocity that is based on concentration and applied stress field. The concentration field is obtained by solving diffusion equation with curvature dependent interface boundary condition and a source term that is a function of effective plastic deformation. The stress field is obtained by solving equations of solid mechanics combined with flow rule and hardening law. The use of fixed grid requires a ghost boundary approach for solving equations over an irregular void boundary. The rate of growth of voids can be determined by analyzing void geometry at each time step using techniques of image processing, which otherwise is difficult to determine analytically for the case of multiple voids. In addition to lower dimensions, the numerical model has also been implemented for multiple voids in three-dimension making it possible to study dynamic fracture of real materials.

11:45 AM AA3.11
Energy Dissipation During Intermediate Strain Rate Deformation in Metals. Wendelin J. Wright[1], Michael W. Burke[2], Wayne O. Miller[2], Michael W. McElfresh[2] and Steven J. DeTeresa[2]; [1]Materials Science and Engineering, Stanford University, Stanford, California; [2]Lawrence Livermore National Laboratory, Livermore, California.

The goal of this work is to study the fraction of plastic work that is dissipated as heat during dynamic deformation and failure of materials. Understanding this partitioning of energy is critical to predicting material response, namely the temperature rise and subsequent softening, localization, and failure that can occur under dynamic loading. Simulations of heat flow during uniaxial compression of aluminum and tantalum at strain rates of 14 s^{-1} indicate that adiabatic conditions are achieved, so that a single point temperature measurement made at the sample surface is a valid measure of the temperature increase. Fine gage thermocouples spot-welded to the surfaces of metallic specimens demonstrate a sufficient response time for accurately capturing the temperature rise during deformation. The fraction of plastic work dissipated as heat is related to the work hardening rate and may be considerably less than 1.0 for metals depending on the work hardening characteristics.

SESSION AA4: Dislocations
Chair: W. Curtin
Tuesday Afternoon, November 29, 2005
Republic B (Sheraton)

1:30 PM *AA4.1
Discrete Discrete Dislocation Modeling of Fracture Processes. Alan Needleman, Brown University, Providence, Rhode Island.

In joint work with V.S. Deshpande of Cambridge University and E. Van der Giessen of the University of Groningen a framework has been developed for the analysis of crack growth where plastic flow arises from the motion of large numbers of discrete dislocations and the fracture properties are embedded in a cohesive surface constitutive relation. The material model is independent of the presence of a crack and the only distinction between an analysis of monotonic crack growth and fatigue crack growth is that in fatigue the remote loading is specified to be an oscillating function of time. Discrete dislocation modeling of various fracture processes, under both monotonic and cyclic loading conditions, will be discussed with a focus on fracture in two-phase materials, i.e. along interfaces and through or around second phase consituents.

2:00 PM AA4.2
Evaluation of the Dislocation Arrangement Near the Crack Tip Region of 316LN Stainless Steel by Neutron Diffraction. Yinan Sun[1], Rozaliya Barabash[2], Hahn Choo[1,2], Peter Liaw[1], Yulin Lu[1] and Don Brown[3]; [1]University of Tennessee, Knoxville, Tennessee; [2]Oak Ridge National Laboratory, Oak Ridge, Tennessee; [3]Los Alamos National Laboratory, Los Alamos, New Mexico.

The deformation in the vicinity of the crack tip was studied with neutron diffraction. Anisotropic line broadening was observed at different distances from the crack tip. The dislocation density and arrangement were studied from the line-width and profile behavior for several crystallographic families. Lattice strains were analyzed by the Rietveld-refinement technique using the General Structure Analysis System (GSAS).The comparison of the results obtained with GSAS and line-profile analysis facilitate the understanding the change of dislocation densities and strains in the plastic zone. The orientation dependence of both strain and line broadening on (hkl) was observed, which indicates the non-random dislocation arrangement. The dislocation density was found to decrease with the distance from the crack tip.

2:15 PM AA4.3
Discrete Dislocation Dynamics Simulation of Plasticity in Small Systems. Meijie Tang, Lawrence Livermore National

Laboratory, Livermore, California.

Recently, we developed a hybrid method for computing forces on curved dislocations threading to free surfaces [Tang et al., 2005] in dislocation dynamics simulations. In the hybrid method, we separate the treatment of the singular and non-singular part of the image stresses. It was shown to be an accurate and efficient way to capture the important image stress effect on dislocation behavior in small systems. The method is further examined in terms of its applicability in complex geometries. Applications are made using this method to study both unit mechanisms and collective behavior of dislocations in finite systems where the free surface and the associated image stresses seem to play a role in the physics of plasticity in small systems. The work is performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48. Meijie Tang, Wei Cai, Guanshui Xu, Vasily V. Bulatov, JMPS, submitted (2005).

3:30 PM AA4.4
In-Situ TEM Observations of Dislocation-Particle Interactions during Elevated Temperature Deformation of Particle-Strengthened Al Alloys. Blythe Gore Clark and Ian M. Robertson; Materials Science and Engineering, University of Illinois, Urbana-Champaign, Urbana, Illinois.

Understanding the macroscopic behavior of a material requires knowledge of the microstructural dynamics occurring during deformation. For particle-strengthened aluminum alloys, deformation is largely controlled by dislocation-particle interactions. Real time observation of these interactions can be obtained via in-situ TEM techniques. Using a combination of in-situ TEM deformation experiments and high resolution imaging, the elevated temperature behavior of particle-strengthened Al-Sc, Al-Mg-Sc, Al-Zr, and Al-Mg-Zr alloys have been compared. In-situ observations of interactions between dislocations and coherent and semi-coherent Al_3Sc and coherent Al_3Zr indicate a change in the nature of the interaction as a function of temperature, particle coherency, and particle size. These observations will be presented, along with elevated temperature bulk compression data, providing insight into the controlling mechanisms occurring during elevated temperature deformation processes, such as creep.

3:45 PM AA4.5
A comparison of debonding and cracking mechanisms in heterogeneous material by discrete dislocations simulation. Sebastien Groh[1], Vickram Deshpande[2], Alan Needleman[1] and Erik Van der Giessen[3]; [1]Engineering, Brown University, Providence, Rhode Island; [2]Engineering, Cambridge University, Cambridge, United Kingdom; [3]Applied Physic, University of Groningen, Groningen, Netherlands.

The understanding of the correlation between microstructure, deformation and damage development in heterogeneous materials is of major importance for engineering materials. The failure of heterogeneous material can result from various failure mechanisms such as: particle cracking, matrix cracking or interface debonding. The competition between these mechanisms is investigated using 2D discrete dislocation simulations in which dislocations are represented by line singularities in an otherwise isotropic linear elastic medium. In addition, fracture is modeled using a cohesive surface framework with different fracture properties for the matrix, the particle and the interface. Initially, a main crack perpendicular to the interface is in the matrix. As the remote loading is increased, the crack reaches the interface and then may penetrate the particle or/and be deflected into the interface depending of the strength of the interface compared to the strength of the particle. The competition between penetration into the particle and debonding of the interface is investigated with a focus on the effects of: (i) the strength of the particle as compared with the strength of the interface; (ii) the dislocation density; and (iii) the particle size.

4:00 PM AA4.6
Multiscale Study of FCC Bicrystals Deformation: Discrete Dislocation Dynamics and Continuum Gradient Crystal Plasticity. Firas Akasheh[1], Hussein Zbib[1] and Tetsuya Ohashi[2]; [1]Mechanical and Materials Engineering, Washington State University, Pullman, Washington; [2]Mechanical Engineering, Kitami Institute of Technology, Kitami, Japan.

The micromechanics of bicrystals deformation is of great interest for the current efforts to develop continuum crystal plasticity models that are more physics-based that are better capable of predicting the observed size dependant response of crystals on the micro scale. Furthermore, bicystals gain particular interest because they also serve as an idealized prototype model for the study of grain boundaries and their effect on the deformation of polycrystals. This work is an attempt along those efforts with particular focus on developing continuum models to describe the role of grain boundaries on mechanical response of polycrystals. Our approach is one of multiscale. On the micro scale discrete dislocation dynamics (DD) is used to simulate the physical behavior of dislocations as they interact with the bicrystal interface under the effect of the associated image forces. On the macroscale, a small strain crystal plasticity model, where dislocations are described as field densities, is used to simulate the same problem as that in DD. The evolution of dislocation densities, structure, as well as the mechanical response from both scales are compared. The parameters of the continuum model are fitted based on the results from DD, which is considered as the reference for comparison.

4:15 PM AA4.7
A Discrete Theory of Dislocation Dynamics in Crystals. Ashwin Ramasubramaniam, M. P. Ariza and M. Ortiz; California Institute of Technology, Pasadena, California.

We present a study of 3D dislocation dynamics in BCC crystals based on discrete crystal elasticity. Ideas are borrowed from discrete differential calculus and algebraic geometry to construct a mechanics of discrete lattices. The notion of lattice complexes provides a convenient means of manipulating forms and fields defined over the crystal. Atomic interactions are accounted for via linearized embedded atom potentials thus allowing for the application of efficient fast Fourier transforms. Dislocations are treated within the theory as energy minimizing structures that lead to locally lattice-invariant but globally incompatible eigendeformations. The discrete nature of the theory automatically eliminates the need for core cutoffs. The quantization of slip to integer multiples of the Burgers vector along each slip system leads to a large integer optimization problem. We suggest a new method for solving this NP–hard optimization problem and present numerical calculations that illustrate the potential of our approach for the simulation of large 3D systems.

4:30 PM AA4.8
Modeling Large Dislocation System: Discrete Dynamics Simulations and Statistical Mechanics Approach. Jie Deng and Anter El-Azab; Mechanical Engineering, Florida State University, Tallahassee, Florida.

Plastic distortion of metals is characterized by complex dislocation dynamics and interactions that give rise to a rich variety of mesoscale dislocation structures. Many models developed to study dislocation patterning have been developed but they are either too simple to capture the three dimensional character of transport and reactions of dislocations or not adequately structured to handle the long range reactions. We summarize a three dimensional statistical mechanics based model for dislocation dynamics and mesoscale plasticity of a single crystal, which allows for simultaneous prediction of the mesoscale distortion of the crystal, dislocation structure, internal elastic fields, and the macroscopic constitutive response of single crystals. We present a numerical solution of this model, and compare the results with those obtained using discrete dislocation dynamics simulation codes.

4:45 PM AA4.9
Stochastic dislocation dynamics through sessile and glissile local potentials. Masato Hiratani, CMS/MSTD, Lawrence Livermore National Laboratory, Livermore, California.

Thermally activated dislocation motion through various local barriers is investigated computationally. Langevin and Brownian discrete dislocation dynamics (DD) schemes are employed to simulate a sequence of thermal activated jumps from metastable configurations and passages between them. The simulation cell size typically ranges from 0.5 to 2 micron, and the total time from 0.5 to 10 ns. In creep simulations of the diluted alloyed copper, a percolation of partial dislocations through sessile local precipitates is found to be a highly non-Arrhenius at a higher stress and low temperature range due to the kinetic energy transfer between the activation site. In constant strain rate simulations of aluminum with mobile precipitates, Portevin-LeChatelier type intermittent behavior is observed in the time series of stress data. Dynamics of a screw dislocation through periodic Peierls potentials is also studied for molybdenum. Horizontal and vertical roughening of dislocation shape is observed due to fluctuation of populations of kinks nucleated on the primary planes and cross-kinks on the secondary planes. Obtained statistical data is used to develop further coarse-grained mobility laws for a deterministic DD model, Parallel Dislocation Simulator (ParaDiS), designed in LLNL to simulate plastic response of a large dislocation ensemble. This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48, and the support of the DOE (Grant No. DE-FG03-01ER54629).

SESSION AA5: Size Effects and Nanomaterials
Chair: W. Curtin
Wednesday Morning, November 30, 2005
Republic B (Sheraton)

8:00 AM AA5.1
Specimen size effect on mechanical properties of ultra-fine grained materials. Yonghao Zhao[1], Yuntian Zhu[1], Cheng Xu[2] and Terry G. Langdon[2]; [1]MST, Los Alamos National Lab., Los Alamos, New Mexico; [2]Departments of Aerospace & Mechanical Engineering and Materials Science, University of Southern California, Los Angeles, California.

Ultra-fine grained Cu was prepared by equal-channel angular pressing (ECAP) in route Bc for six passes. Bone-shaped specimens for mechanical test were produced with different thicknesses and gauge lengths. It was found that the ductility (tensile elongation to failure) decreases with decreasing the thickness, while increases with decreasing the gauge length. The yield strength did not change significantly against the thickness and gauge length. Moreover, with decreasing the specimen thickness, the fracture mode changed from ductile necking to shear breaking. The origin of the specimen thickness and length effects on the ductility and fracture of the ultra-fine grained materials will be discussed.

8:15 AM AA5.2
Mechanical Properties of Free-Standing Single Crystal Gold Nanowires. Jeffrey William Kysar, Dongyun Lee and James Hone; Mechanical Engineering, Columbia University, New York, New York.

The mechanical properties of free-standing nanowires consisting of single crystal gold are studied experimentally. The specimens are fabricated from pure gold leaf with an approximate thickness of 100 nm to 150 nm which is attached to a silicon substrate. The in-plane grain size of the leaf as investigated with Electron Backscatter Diffraction (EBSD) is of the order of tens of microns. Specimens suitable for mechanical testing are fabricated within individual grains of the leaf via standard lithographic techniques. The final specimen is in the form of a "dog bone". The ends of the specimen are anchored to the silicon substrate and the silicon below the gauge section is etched away, which results in a free-standing gauge section. The gauge length of the specimen is eight micrometers and the cross-sectional dimensions of the gauge length are about 150 nm by 200 nm. Importantly, the residual stress in the specimen is negligible. The mechanical properties of the single crystal gold are probed by deflecting the gauge section with a nanoindenter. The resulting stress-strain curve is serrated and the material can have a yield stress approaching 1 GPa. The deformation is localized in slip bands characteristic of plastic flow in single crystals.

8:30 AM AA5.3
Plasticity and Fracture of Micro-pillars and Nanowires. Wei Cai, Christopher R. Weinberger and Keonwook Kang; Mechanial Engineering, Stanford University, Stanford, California.

The deformation of semiconductor nanowires under tension and metal micro-pillars under compression are studied using atomistic and micromechanical models. The emphasis is on the effect of the confining geometry on the nucleation, migration and interaction of lattice defects, e.g. dislocations and cracks. The cylindrical geometry of both systems permits a common treatment in micromechanical models based on continuum elasticity theory. The results will be compared with experiments to elucidate the mechanism of transition in the mechanical behavior as the cylinder diameter decreases from micrometer to nanometer regime.

8:45 AM AA5.4
Size Matters: Tiny Gold Pillars as Strong as Steel. Julia Rosolovsky Greer and William D. Nix; Materials Science and Engineering, Stanford University, Stanford, California.

The results of both experimental studies and molecular dynamics simulations indicate that crystals exhibit strong size effects at the sub-micron scale. In experimental studies, the size effects are usually explained by the presence of strain gradients. One of the more prominent strain gradient plasticity theories was developed by Nix and Gao. While this model accurately predicts the observed increase in hardness as the deformation volume decreases, it fails to describe the discrete behavior indicative of nucleation of dislocations at the indentation depths shallower than ∼100nm. By contrast, more recent experiments and some molecular dynamics (MD) simulations suggest that the yield strength of crystalline materials depends on the specimen size even without strain gradients and scales with the sample size through a power relationship. In the scope of this work, results of uniaxial compression experiments of free-standing gold single-crystalline and poly-crystalline nanopillars without imposing significant stress/strain gradients are presented. These Au cylinders are created by focused ion beam (FIB) machining and by Microlithography/Electroplating techniques. They are subsequently compressed using a Nanoindenter fitted with a custom-fabricated diamond flat punch. Compressive stresses and strains, as well as pillar stiffnesses are determined from the test data. The experiments show that the flow stresses of these pillars increase significantly with decreasing pillar volume, reaching stresses as high as 0.8 GPa for the smallest pillars. These results indicate a 50x flow stress increase compared to that of bulk gold which is reported to be ∼20 MPa at 2% strain. These high strengths appear to be controlled by dislocation starvation, unique to very small crystals. TEM studies and dislocation starvation model results are discussed.

9:00 AM AA5.5
Micron-Scale Plasticity in Single Crystalline Au and Mo. Christoph Eberl and Kevin J. Hemker; Mechanical Engineering, Johns Hopkins University, Baltimore, Maryland.

Size effects have been shown to play a crucial role in the plastic behavior of metals and alloys, and efforts to understand and model the plastic response in restricted sample volumes have received renewed attention in recent years. The renewal is fueled, at least in part, by the availability of micromachining tools that enable sample preparation on the micrometer scale. To date, the vast majority experiments have involved micro-compression testing. In this paper the preparation, conduction and analysis of tensile tests on the micron scale will be presented. Thin slices of single crystalline Au and Mo have been electro-polished and pre-shaped into MEMS inspired specimens by use of a micro electrode discharge machine. The final gage sections are formed with judicious use of focused ion beam machining. Micro-tensile testing is conducted using a piezo driven actuator, an in-line load cell and displacement control. The strain at the gage section is measured by the use of optical digital image correlation and the as-deformed samples are analyzed by SEM, FIB and TEM with emphasis on the characterization of dislocation microstructures. The micro-tensile behavior will be compared and contrasted with the size effects recently reported for micro-compression experiments, and the observed plasticity will be discussed considering proposed models for Hall-Petch behavior and dislocation starvation.

9:15 AM AA5.6
Strain-gradient Plasticity Modeling of Length-scale and Bauschinger Effects in Thin-film Plasticity. Yong Xiang and Joost J. Vlassak; Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts.

Recent experiments on passivated freestanding thin Cu films reveal large length-scale and Bauschinger effects in the plastic deformation of very thin metal films. Classical plasticity theories do not provide an adequate description of these observations. Several classes of strain-gradient plasticity theories have recently been proposed to explain the thickness effect associated with small-scale plasticity. These models predict the length-scale effects in certain experimental configurations, but do not capture the observed Bauschinger effect very well. Thus far, few attempts have been made to measure and explain the Bauschinger effect in thin films and most comparisons are made only between theoretical models and discrete dislocation simulations. In this work, we propose a new strain-gradient plasticity theory that captures both the length-scale and Bauschinger effects in thin film plasticity. The model is based on the stretch and rotation version of the strain-gradient plasticity theory developed by Fleck and Hutchinson. The isotropic and kinematic contribution to the total hardening are separated and expressed in terms of the plastic strains and their gradients. The strengthening is a sum of both isotropic and kinematic hardening; while the Bauschinger effect is related to the back stresses associated with kinematic hardening. By fitting the model to our experimental data for thin Cu films, the length scale associated with the strengthening effects in these films is found to agree well with values in the literature. At the same time, the thickness-dependent Bauschinger effect can be explained as the result of back stresses that are functions of both the plastic strains and their gradients.

10:00 AM AA5.7
Mechanical and Fracture Properties of Micro-sized Bending Beams Machined by the Focused Ion Beam Technique. Christian Motz, Thomas Schoeberl and Reinhard Pippan; Erich Schmid Institute, Austrian Academy of Sciences, Leoben, Austria.

Micro-sized bending beams with thicknesses, t, from 7.5 down to 1.0 μm were fabricated with the focused ion beam technique from copper and tungsten single crystals with an {111}<011> and an {011}<111> orientation, respectively. The beams were loaded with a nano-indenter and the force vs. displacement curves were recorded. A strong size effect was found, where for the thinnest beams the flow stresses reach almost 1 GPa for copper and 7 GPa for tungsten. A

common strain gradient plasticity approach was used to explain the size effect. However, the strong t-1.14 dependence of the flow stress could not be explained by this model. Additionally, the combination of two other dislocation mechanisms is discussed: the limitation of available dislocation sources and a dislocation pile-up at the beam centre. The contribution of the pile-up stress to the flow stress gives a t-1 dependence, which is in good agreement with the experimental results. Additionally, fracture tests were performed on the tungsten beams. The tungsten beams were notched using the focussed ion beam, which gives a sharp notch with tip radii of a few nanometers. Subsequently, the beams were fractured with the use of a nano-indenter and the load vs. displacement response was recorded. The configuration is similar to three point bending tests and fracture toughness values, K_IC, are estimated. Furthermore, the fracture surfaces are investigated with a scanning electron microscope. The resulting fracture toughness values and the fracture surfaces are compared with the macroscopic behaviour.

10:15 AM AA5.8
Discrete Dislocation Plasticity of Gradient-Free Size Effects.
Vikram S. Deshpande[2], Alan Needleman[3] and Erik Van der Giessen[1]; [1]Materials Science Center, University of Groningen, Groningen, Netherlands; [2]Engineering Department, University of Cambridge, Cambridge, United Kingdom; [3]Division of Engineering, Brown University, Providence, Rhode Island.

During the last decade, a variety of models have been developed to help understand size effects of the type 'smaller is harder' seen in experiments such as bending, torsion and indentation. The key to these size effects lies in the presence or development of gradients in plastic strain. Discrete dislocation formulations and also a few strain gradient plasticity theories have been developed that pick-up the effects, because they are embodied with one or more material length scales. Recent experiments by, e.g., Nix and Dimiduk on micron-sized pillars under compression have provided an additional challenge for modeling: size effects in the absence of strain gradients. Here we present results of two-dimensional discrete dislocation simulations of single crystals under tension and compression that reveal a distinct size effect with smaller being stronger. The findings for either single and double slip suggest that 'dislocation starvation' is at the origin of the effect, and we explore the effect of nucleation strength and distribution. Also we discuss the influence of initially frozen-in dislocations.

10:30 AM AA5.9
Simulation of Size Effects using 2D Dislocation Dynamics.
Sidonie Lefebvre[1,2], Benoit Devincre[3] and Thierry Hoc[1]; [1]MSSMAT, Ecole Centrale Paris, Chatenay Malabry, France; [2]Altissemiconductor, Corbeil Essonne, France; [3]LEM, CNRS-Onera, Chatillon, France.

Miniaturizing microelectronic components is a necessity for the semiconductor industry, but this involves reliability issues. This is especially the case for FCC polycrystalline freestanding films and interconnects, with a grain size d between 200 nm and a few microns. Such ultrafine-grained microstructures have attracted a wealth of interest in recent years, as their mechanical properties drastically differ from those of bulk materials. From a micromechanical viewpoint, two types of boundary value problems must be distinguished at grain level. One can have either grains in the bulk, bounded by grain boundaries (GBs), or grains also bounded by free surfaces or interphases (e.g. columnar grains in epitaxial layers). For the sake of simplicity, only the former case is considered here. In bulk conditions, experiments on copper polycrystal show that the grain size dependence of the yield stress follows a Hall Petch law down to grain sizes less than 100 nm in clean materials. Departures from the Hall Petch relation are unavoidable at very small grain sizes, but their experimental observation depends on how the materials have been processed. Further, whether or not the yield stress of polycrystalline thin films and small-size samples like interconnects follow a d^{-1} or a $d^{-1/2}$ dependence, is still a matter of debate. Plastic deformation is strongly heterogeneous at the micrometric scale. Hence, conventional constitutive formulations are no longer appropriate in this domain. Mesoscopic simulations of dislocation dynamics (DD), which describe the motion and interactions of dislocations are, in contrast, quite suited for studying this type of problem. In this work, we investigated the ability of DD simulations to reproduce size effects in ultra-fine grained fcc polycrystals. The evolution of the yield and flow stress in polycrystals with characteristic grain sizes ranging from 2 μm down to 500 nm is studied by two-dimensional dislocation dynamics simulations. The results obtained are consistent with a Hall Petch relationship. In addition, a linear relation is found between the rate of increase of the dislocation density and the inverse of the grain size. As a consequence, the size effect in this grain size range is found to be governed by the reduction in dislocation mean-free path induced by grain boundaries rather than by dislocation nucleation. Moreover, the DD results showed that size reduction leads to a homogeneous glide on slip systems and a strong difference in internal stress field.

10:45 AM AA5.10
A Cellular Automaton Model of Size Effects in Micropillar Samples.
Peter M. Anderson[1], Julia R. Greer[2] and William D. Nix[2]; [1]Materials Science and Engineering, Ohio State University, Columbus, Ohio; [2]Materials Science and Engineering, Stanford University, Stanford, California.

Recent compression testing of gold pillars with submicron diameters shows flow strengths as large as 50 times that of bulk counterparts. Corresponding transmission electron microscopy of deformed pillars reveals small dislocation densities, suggesting that such large strengths cannot be explained via traditional strain hardening concepts. Stress-strain traces at uniform strain rate show a rapid build-up to a peak stress, followed by repeated release and build-up of stress. A cellular-automaton model is proposed to determine if these results can be explained by the evolution of dislocation content inside a deforming micropillar. The model is based on discretizing pillars into cells with prescribed initial dislocation density and distribution of dislocation source lengths. The dislocation density in each cell evolves due to source operation, dislocation breeding, exchange of dislocation content, and load shedding. Smaller pillars are inherently different due a distribution of source lengths that is truncated by the pillar size and also the inability to contain bursts of dislocation activity. The model predictions and assumptions are assessed in light of recent experimental stress-strain data.

11:00 AM AA5.11
Hierarchical Modeling of Failure Mechanisms and Grain-Boundary Effects in Nanocrystalline Aggregates.
Toshirio Kameda, Mohammed A. Zikry, A. M. Rajendran, Donald Brenner, W. M. Ashmawi and Fadi Abdeljawad; Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, NC, North Carolina.

New computational methodologies have been developed to predict dominant material behavior and mechanisms at scales ranging from the nano to the macro. Physically based scaling relations have been developed to characterize mechanisms and grain-boundary effects. These scaling relations have been used to link molecular dynamic and microstructural modeling to delineate the interrelated effects of grain boundary orientation and structure, dislocation transmission, absorption, and blockage through GBs, and such that dominant failure mechanisms can be accurately identified and predicted from initiation to unstable growth.

11:15 AM AA5.12
Deformation Mechanisms of Nanocrystalline Materials under Cyclic Loading.
Diana Farkas, Materials Science, Virginia Tech, Blacksburg, Virginia.

The mechanisms of fatigue behavior in nano-crystalline metals were investigated at the atomic scale using empirical force laws and molecular level simulations. A combination of molecular statics and molecular dynamics was used to deal with the time scale limitations of molecular dynamics. The main atomistic mechanism of fatigue crack propagation in these materials is the formation of nano-voids ahead of the main crack. The results obtained for crack advance a a function of stress intensity amplitude are consistent with experimental studies and a Paris law exponent of about 2. The results are discussed in comparison to deformation mechanisms in nanocrystalline materials under monotonic loading.

11:30 AM AA5.13
Molecular-Dynamics Parameterization of a Cohesive Zone Model for Intergranular Fracture in Aluminum.
Vesselin I. Yamakov[1,3], Dawn R. Phillips[2,3], Erik Saether[3] and Edward H. Glaessgen[3]; [1]National Institute of Aerospace, Hampton, Virginia; [2]Lockheed Martin Space Operations, Hampton, Virginia; [3]NASA Langley Research Center, Hampton, Virginia.

A traction-displacement relationship that characterizes the load transfer across a growing nanoscopic intergranular crack is extracted from atomistic molecular dynamics simulations and is recast in a form that is suitable for inclusion within continuum finite element models. In this study, a molecular-dynamics model for crack propagation under steady-state conditions is developed to analyze inter-granular fracture along a flat $\Sigma 99$ [1 1 0] symmetric tilt grain boundary in aluminum. Under hydrostatic tensile load, the simulation reveals asymmetric crack propagation in the two opposite directions along the grain boundary. In one direction, the crack propagates in a brittle manner by cleavage with no or very little dislocation emission, and in the other direction, the propagation is ductile through the mechanism of deformation twinning. This behavior is well explained by the Rice criterion (Rice, J. R., J. Mech. Phys. Solids 40, 1992, 239-271) for cleavage vs. dislocation blunting transition at the crack tip, and the preference for twinning to dislocation slip is in agreement with the

Tadmor and Hai criterion (Tadmor, E. B. and Hai, S., J. Mech. Phys. Solids 51, 2003, 765-793). A comparison with finite element calculations shows that while the stress field around the brittle crack tip follows the expected elastic solution for the given boundary conditions of the model, the stress field around the twinning crack tip has a strong plastic contribution. Through the definition of a cohesive-zone-volume-element - an atomistic analog to a continuum cohesive zone model element - the results from the molecular-dynamics simulation are recast to obtain an averaged continuum traction-displacement relationship that represents the cohesive interactions along a characteristic length of the grain boundary interface for the case of ductile and brittle decohesion.

SESSION AA6: Nanomaterials
Chair: Y. Qi
Wednesday Afternoon, November 30, 2005
Republic B (Sheraton)

1:30 PM *AA6.1
A Continuum model for shock-loaded nanocrystalline metals.
Raul Radovitzky, MIT, Cambridge, Massachusetts.

Recent molecular dynamics simulations of shock-loaded nanocrystalline copper have shown unprecedently high strength behind the shock front accompanied by a reduction of grain boundary sliding and other deformation mechanisms, suggesting that the softening effect of grain boundaries at the nanoscale is curtailed by grain boundary compression. In this presentation, I describe a continuum approach trying to capture this unique aspect of the mechanical response of nanocrystalline copper under shock loading. I will describe the main elements enabling the continuum simulation of intense shocks propagating in nanocrystals including a continuum description of sliding and accommodation at grain boundaries, a polyconvex model of the deviatoric anisotropic elastic response, the integration of an equation of state obtained from ab initio calculations, the integration with multiscale models of crystal plasticity, the numerical need for specialized shock-capturing methods and, finally, the need for a computational framework for conducting high-resolution, large-scale calculations of the resulting initial boundary value problem. I will present simulations that attempt to reproduce the MD results and comment on their success in describing the basic deformation features predicted by atomistic descriptions.

2:00 PM AA6.2
Dynamic Flow Localization in Commercial Purity Tungsten with Ultrafine Grained and Nanocrystalline Microstructures.
Qiuming Wei[1,2], Brian H. Schuster[3,2], Kaliat T. Ramesh[2], En Ma[2], Laszlo J. Kecskes[3], Robert J. Dowding[3], Kyu Cho[3] and Ruslan Z. Valiev[4]; [1]Mechanical Engineering and Engineering Science, University of North Carolina at Charlotte, Charlotte, North Carolina; [2]CAMCS, The Johns Hopkins University, Baltimore, Maryland; [3]US Army Research Lab, Aberdeen Proving Ground, Maryland; [4]Ufa State Aviation University, Ufa, Russian Federation.

Flow localization in the form of adiabatic shear bands and the subsequent failure has long been a desired deformation and failure mode for some critical applications. For example, in the past several decades tremendous effort has been exercised (but with little success) to produce tungsten that possesses such behavior. We report in this work dynamic flow localization under uni-axial compression in commercial purity tungsten that is driven by ultrafine grained (UFG) and nanocrystalline (nc) microstructures. We use severe plastic deformation (SPD) to refine the grain size of a coarse-grained tungsten into the UFG/nc regimes. Such microstructures exhibit much elevated strength, vanishing strain hardening, and much reduced strain rate sensitivity, which work together to render the material much more prone to adiabatic shear banding.

2:15 PM AA6.3
Direct measurement of elastic properties of silica nanowires.
Emilio C. Silva[1], Sidney Yip[1,2] and Krystyn J. Van Vliet[1]; [1]Department of Materials Science & Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; [2]Department of Nuclear Science & Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Nanostructures are posited and sometimes demonstrated to exhibit unique mechanical properties, such as high tensile strength. However, experimentally obtaining these mechanical properties remains challenging due to the small material dimensions and correspondingly small loads and displacements. Here, we report the bending stiffness of cantilever silica wires with diameters ranging from the micro- to the nanoscale, using an atomic force microscope to apply transverse loads at different points on the wire. Silica is considered a model geomaterial for which the mechanisms of moisture-induced mechanical degradation are important but poorly understood. While similar mechanical characterization of carbon nanotubes, silicon carbide, gold and silver nanowires has been reported, the stiffness of silica nanowires was heretofore available only through indirect measurements. For diameters between 250 nm and 2 μm, the Young's modulus of the silica wires is consistent with that of bulk silica, within the precision of this method. Classical molecular dynamics simulations using the BKS potential suggest that silica wires of smaller dimensions (less than 10 nm in diameter) will be considerably stiffer than bulk silica. This technique holds great promise for understanding the mechanical behavior of covalently bonded, networked nanostructures for which mechanical properties depend strongly on environmental interactions.

3:30 PM *AA6.4
Stress Dependence of Microstructural Changes in Carbon Nanotube Reinforced Composites and Silicon.
Liangchi Zhang, School of Aerospace, Mechanical & Mechatronic Engineering, The University of Sydney, Sydney, New South Wales, Australia.

Carbon nanotubes and monocrystalline silicon are two important materials to modern industry. This invited presentation will discuss the mechanics of some microstructural changes in silicon and in carbon nanotube reinforced polymer composites induced by external stresses. An emphasis will also be placed on the further research required to clarify some key aspects of the stress dependence of these microstructural changes. The discussion will concentrate on the following two parts: (a) the complicated phase transformations in silicon and their constitutive modelling under the coupled hydrostatic and shear stresses; and (b) the atomic structural re-construction of carbon nanotubes in composites under surface stresses. The mechanics of these problems is explored with the aid of a multi-scale analysis, both theoretically and experimentally, using quantum mechanics, molecular dynamics, continuum mechanics and electron microscopy of atomic resolution. Some findings are briefly given below: It was found that the variation of stresses plays a key role in the phase transformation events. In a single loading cycle with a spherical indenter, the deformed zone can be amorphous, a mixture of crystalline and amorphous, or purely crystalline, depending on the level of the maximum load. Under cyclic loadings, some phases can be activated from the 2nd cycle and result in the formation of a multi-phase composite in the deformed zone whose properties will be stabilized in the subsequent cycles even under a fixed external load. Water has an obvious effect, which changes the local stress field and in turn reduces the quantity of the metallic b-Sn phase. Similarly, because of the difference in stresses generated, a Berkovich indenter creates different distributions of phases and accelerates the process of crystallization. Molecular dynamics and constitutive analysis showed that the stress-dependence can be modelled concisely using the continuum mechanics theory. When carbon nanotubes in polymer was subjected to surface loading and heating, the nanotubes were significantly deformed with microstructural changes, including bonding breakage and cap removing. More interestingly, the nanotubes can re-assemble its atomic structure. A systematic experimental examination and a combined quantum mechanics and molecular dynamics analysis showed that when the bonding between the nanotubes and polymer matrix was strong, more re-assembled structures would be produced.

4:00 PM AA6.5
Nanoindentation and Microstructural Evolution in Crystalline Materials.
Jeong Beom Ma, Mohammed A. Zikry, Waeil M. Ashmawi and Donald Brenner; Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, NC, North Carolina.

Specialized large-scale computational finite-element have been coupled with molecular dynamic models to understand and predict how dislocation density emission and contact stress fields due to nanoindentation affect inelastic deformation evolution at scales that span the molecular to the continuum level in ductile crystalline systems. Dislocation density distributions and local stress fields have been obtained for different crystalline slip-system and grain-boundary orientations. The interrelated effects of grain-boundary interfaces and orientations, dislocation density evolution and crystalline structure on indentation inelastic regions have been investigated and correlated with different experimental observations and measurements.

4:15 PM AA6.6
Simulations of Strength and Fracture in Amorphous and Nanostructured Carbon.
Maria G. Fyta[1], Ioannis N. Remediakis[1], Pantelis C. Kelires[1] and Dimitrios A. Papaconstantopoulos[2]; [1]Physics Department, University of Crete, Heraclion, Greece; [2]Naval Research Laboratory, Washington, District of Columbia.

Carbon-based materials are considered to be excellent candidates for extreme hardness and thermal stability, approaching those of diamond. This class of materials includes single-phase tetrahedral amorphous carbon (ta-C), with a high fraction of sp$\hat{3}$ hybrids,

nanocomposite carbon, in which diamond nanocrystallites are embedded in a-C, and nanodiamond films with disordered, sp$\hat{2}$-rich grain boundaries. Despite the importance of these systems for MEMS/NEMS devices and ultrahard coatings, several critical aspects of their strength and deformation properties remain elusive. Some of the fundamental issues are: (a) The elucidation of fracture mechanisms in ta-C and nanostructured C. For the latter, one asks whether fracture occur inter- or intra-grain. (b) The explanation of why ta-C is measured to have high hardness ($\sim$ 50-80 GPa) but still lower than diamond's ($\sim$ 100 GPa), despite the absence of easy-slip (cleavage) planes. (c) The question whether nanoinclusions improve the elastic moduli and strength of ta-C. We present here the results of state-of-the-art tight-binding (TB)molecular dynamics simulations, using the NRL TB code, which shed light into these fundamental issues. For the first time, we identify the fracture mechanisms in both ta-C and nanocomposite C. We show that the onset of fracture in ta-C takes place at weakly bonded sp$\hat{3}$ sites, which are under tension and spatially associated with clustered sp$\hat{2}$ sites. The C-C bond in the amorphous network, even for a hypothetical 100% sp$\hat{3}$ structure, is weaker than in diamond due to the medium range dihedral angle disorder. A remarkable finding is that in the nanocomposites fracture under tensile or shear load occurs inter-grain, in the embedding matrix, which limits the strength to that of ta-C. However, the elastic moduli are significantly enhanced. We are currently examining whether fracture in ultra-nanocrystalline diamond films occurs as propagation of microcracks in the grain boundaries or intra-grain.

4:30 PM AA6.7
Stress enhancement and fracture toughness in nanostructured silicon carbide. Luciano Colombo[1,3], Mariella Ippolito[1,3], Alessandro Mattoni[1,3] and Fabrizio Cleri[2]; [1]Department of Physics, University of Cagliari, Monserrato (Ca), Italy; [2]Unita' Materiali e Nuove Tecnologie, ENEA, C.R. Casaccia (Roma), Italy; [3]Sardinian Laboratory for Computational Materials Science (SLACS), CNR/INFM, Monserrato (Ca), Italy.

By using atomistic simulations, we derive a constitutive equation for a microfractured β-SiC matrix containing hard or soft inclusions. Present simulations are performed by constrant-traction border conditions, that proved to correctly represent mechanical loads on atom-resolved nanostructured systems.[1] The proposed equation is shown to follow the Eshelby theory for elastic inclusions, and appears to hold for any crack tip-inclusion distance, and for a wide range of values of matrix-inclusion elastic mismatch.[2] A comparison of the atomistic results with existing continuum elasticity models [2,3] points out the weaknesses of some commonly adopted simplifying assumptions. [1] A. Mattoni, L. Colombo, F. Cleri, Phys. Rev. B {70}, 044108 (2004) [2] M. Ippolito, A. Mattoni, L. Colombo, F. Cleri, submitted for publication (2005) [3] J. Helsing, Engng. Fracture Mech. {64}, 245 (1999) [4] Z. Li and Q. Chen, Engng. Fracture Mech. {70}, 581 (2003)

4:45 PM AA6.8
Differences in Deformation and Fracture Mechanisms Between Al-Si Nanocomposites with Al Nano-Crystals: A Molecular Dynamics Study. D. K. Ward[1], W. A. Curtin[1] and Yue Qi[2]; [1]Solid Mechanics, Brown University, Providence, Rhode Island; [2]General Motors, Warren, Michigan.

Molecular Dynamics in conjunction with Modified Embedded Atom Method is used to examine the deformation and failure of polycrystals consisting of Al and Si nanograins loaded in tension with a strain rate of 1%/20ps at 300K. Polycrystals that contain eight hexagonal grains of 5nm diameter with [011]-oriented columnar grains with zero, one, or two Si particles are examined to understand the effect of Si additions on the deformation and failure of the material. Using similarly oriented grains with increasing Si content we show that the elastic response is stiffened by the presence of Si particles. Early stages of inelasticity for an Al polycrystal and low Si content nanocomposite show similar stress-strain responses but different mechanisms dominate the deformation. The Al polycrystal shows a mix of grain boundary deformation and dislocation activity while the Al-Si polycrystals show significant grain boundary sliding/shearing only at the Al-Si interfaces with far less activity within the Al. The grain boundary sliding/shearing in the Al-Si nanocomposite is also reduced with increasing Si content, leading to higher yield stresses. The failure modes also differ between the polycrystal and the nanocomposite, failure in the Al polycrystal exhibit two failure modes: fracture-like failure and severe shearing leading to void nucleation. Failure in the Al-Si composites occurs due to localized straining near the Al-Si interface. At remote loads of 2.5-3GPa the localized straining in the nanocomposite leads to debonding at the Al-Si interface but the normal stresses at the interface are $\sim$4 GPa due to stress concentrations from the particle. These local failure stresses have values that are comparable to stresses seen in the failure of biomaterials with the same interfaces. These results suggest that Al-Si nanocomposites have failure dominated by the Al-Si interface and they can be engineered for high strength.

SESSION AA7: Poster Session: Nanocomposites and CNTs
Chair: W. Curtin
Wednesday Evening, November 30, 2005
8:00 PM
Exhibition Hall D (Hynes)

AA7.1
Micromechanics and Macromechanics of Carbon Nanotube Enhanced Elastomers. Sabine Cantournet[1,2], Mary C. Boyce[1] and Andy Tsou[3]; [1]Mechanical Engineering, MIT, Cambridge, Massachusetts; [2]Centre des Materiaux, Ecole des Mines, Paris, Ile de France, France; [3]ExxonMobil, Baytown, Texas.

In this work, the influence of carbon nanotubes on the mechanical behavior of elastomeric materials is investigated. The large deformation stress-strain behavior of an elastomer during uniaxial tension and uniaxial compression is first presented. This elastomer is then enhanced with multi-wall carbon nanotubes (MWCNTs) and the influence of weight fraction (0%, 0.5%, 1%, 2%, 5%, 10%, 15%) of MWCNTs on the large deformation behavior is quantifed. The initial stiffness and subsequent stretch-induced stiffening at large strains are both found to increase with MWCNT content. Surprisingly, not only do the MWCNTs increase the stress at break in tension, but the MWCNTs also increase the tensile stretch at break. In situ x-ray is utilized to monitor the orientation of the MWCNTs with deformation and correlated the evolving orientation with the features of the stress-strain behavior. A constitutive model for the large strain deformation behavior of elastomers is then presented which captures the state of deformation dependence of the stress-strain behavior. The incorporation of the effects of carbon nanotubes on this behavior via a development of a constitutive element which tracks the stretching and rotation of a distribution of wavy carbon nanotubes is then addressed. The dependence of the entire stress-strain behavior on the volume fraction of CNTs is demonstrated. The model is shown to track the stretching and rotation of the CNTs with macroscopic stretch as well as predict the macroscopic stress-strain behavior.

AA7.2
Mechanical behavior of a carbon nanotube turf.
Sinisa Dj. Mesarovic[1], Coralee M. McCarter[1], David F. Bahr[1], Harish Radhakrishnan[1], Robert F. Richards[1], Cecilia D. Richards[1], Devon McClain[2] and Jun Jiao[2]; [1]School of Mechanical and Materials Engineering, Washington State University, Pullman, Washington; [2]Department of Physics, Portland State University, Portland, Oregon.

Exceptional mechanical and thermal properties of carbon nanotubes (CNT) qualify them for many potential applications. Carbon nanotubes grown on a substrate form a turf - a complex structure of intertwined, mostly nominally vertical tubes, cross-linked by adhesive contact and few bracing tubes. The turfs are compliant and good thermal conductors, and thus - a promising thermal contact switch material for MEMS. In this paper, the mechanical behavior of CNT turfs is analyzed and the physical mechanism of deformation deduced on the basis of: (a) experimental results - standard and continuous stiffness nanoindentation tests; and, (b) micromechanical scaling analysis. The material exhibits fully reversible deformation with a small Kelvin-Voigt type relaxation, caused by the thermally activated sliding of contacts. The pre-existing (locked-in) strain energy of bent nanotubes produces a high initial tangent modulus, followed by an order of magnitude decrease in the tangent modulus with increasing deformation.

AA7.3
Structural Mechanic Modeling of Damping Behavior of CNT-Reinforced Composite Materials. Liya Bochkareva, [1]NAS of Belarus, Minsk, Belarus; [2]University of Sheffield, Sheffield, United Kingdom.

A novel concept of nanoparticle vibration damping [1, 2] shows the effect that molecule-level mechanism and friction can have on the damping and nanoparticles/fibres/tubes-reinforced materials can provide enhanced strength and vibration damping properties. It is particularly worth noting that carbon nanotubes and spider silk can act as a simple nanoscale spring with friction-related energy dissipation mechanism. Due to CNT ultra small, nanometer scale size and low density, the surface area to mass ratio (specific area) of carbon nanotubes (CNTs) is extremely large and require extensive investigations for further applications in damping components. There are three types of damping matrix (metal, ceramic and polymer) and in a CNT-reinforced composite material; high damping mechanisms can be achieved via the interfacial friction between the CNT and polymer matrix. Moreover, CNT may offer multifunctionality to the

design of such composites. The purpose of this paper is to establish a platform to investigate the structural damping characteristics of CNT-reinforced composites. The system is modeled using a multi-phase composite. Advanced FEM-based micromechanical model is proposed to describe interfacial damping mechanism evolution. To describe damping effects, the concept of interfacial "stick-slip" frictional motion between nanotubes and polymer is proposed. The analytical results present that critical shear stress, weight ratio and structure deformation is among important factors affecting the damping characteristic in aerospace components. It is also observed that CNT-based composites could achieve higher damping than composites with several other types (different size, surface area, density and stiffness) of fillers. These results confirm the possible advantage of using CNTs for damping enhancement and multifunctional applications.

AA7.4
Exploiting the Nanotube-Polymer Sliding Dissipation Mechanism to Engineer Mechanical Damping in Composite Materials. Jonghwan Suhr and Nikhil A. Koratkar; Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechinc Institute, Troy, New York.

Engineering structural components with high levels of inherent damping is critically important in a variety of aerospace, mechanical, and civil systems. In this study, singlewalled carbon nanotubes and bisphenol-A-polycarbonate composite beams were fabricated by a solution mixing process and dynamic (cyclic) load tests were performed to characterize the damping response. We report an order of magnitude ($> 1000\%$) increase in loss modulus of the polycarbonate system with the addition of 2% weight fraction of oxidized singlewalled carbon nanotube fillers. This is the first time that an order of magnitude change in the damping properties of bulk polymers has been reported, using nanoscale fillers. We show that the increase in energy dissipation is derived from frictional sliding at the nanotube-polymer interfaces. The nanoscale dimensions of the tubes not only results in large interfacial contact area, thereby generating high damping efficiency, but also enables seamless integration into composite structures. This mechanism is far more effective at increasing damping than one based on tube-tube sliding which we have reported previously. The latter mechanism required strong tube-tube contacts, which necessitated a very high packing density of nanotubes, restricting practical applications to thin films. In contrast, the tube-polymer sliding mechanism allows the efficient introduction of damping into bulk polymer structures.

AA7.5
Effects Of Curvature Of The Carbon Nanotubes And Carbon Nanotube/Matrix Bonding On Nanocomposite Stiffnes. Antonio Pantano[1,2], David M. Parks[2], Mary C. Boyce[2], Marco Buongiorno Nardelli[3] and Francesco Cappello[1]; [1]Dipartimento di Meccanica, University of Palermo, Palermo, Italy; [2]Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; [3]Department of Physics, North Carolina State University, Raleigh, North Carolina.

Due to the high stiffness and strength of carbon nanotubes, as well as their ability to act as conductors, carbon nanotubes are under intense investigation as fillers in polymeric materials. The nature of the carbon nanotube/polymer bonding and the curvature of the carbon nanotubes within the polymer have arisen as particular factors in the efficacy of the carbon nanotubes to actually provide any enhanced stiffness or strength to the nanocomposite. Here the effects of carbon nanotube curvature and interface interaction with the matrix on the nanocomposite stiffness are investigated using micromechanical analysis. We recognize and acknowledge poor bond and thus poor shear lag load transfer to the CNT. Therefore Composite Stiffness Enhancement can be achieved through the bending energy of the CNT rather than through the axial stiffness and energy of the CNTs; the bending also best capitalizes on the MWNTs and usage of all internal walls to enhance composite stiffness. A previously-developed nonlinear structural mechanics procedure for modeling mechanical behavior of carbon nanotubes is used [1-4]. The approach realize the extreme computational savings necessary to effectively model CNTs inside the matrix without losing significant accuracy with respect to atomistic methods. Individual tubes are modeled using shell finite elements, where a specific pairing of elastic properties and mechanical thickness of the tube wall is identified to enable successful modeling with shell theory. The effects of non bonded forces generated from the attractive and repulsive forces, due respectively to van der Waals and to Pauli's exclusion principles, are simulated with special interaction elements that are crucial in tube/tube or tube/substrate interactions as well as in maintaining the interwall separation in MWNTs. This new nonlinear structural mechanics based approach for modeling CNTs was verified by comparison with MD simulations and high-resolution micrographs available in the literature [1-4]. Our micromechanical models of curved CNTs within a matrix demonstrate the potential benefit of CNT curvature on nanocomposite stiffness. References [1]. Pantano, A.; Parks, D. M.; Boyce, M. C. Phys. Rev. Lett. 2003, 91, 145504. [2]. Pantano, A.; Boyce, M. C.; Parks, D. M. J. Mech. Phys. Solids 2004, 52, 789. [3]. Pantano, A.; Boyce, M. C.; Parks, D. M. J. of Eng. Materials and Technology, Trans. ASME 2004, 126, 279-284. [4]. Pantano, A.; Parks, D. M.; Boyce, M. C.; Buongiorno Nardelli, M. J. of Applied Physics 2004, 92, 6756-6760.

AA7.6
Abstract Withdrawn

AA7.7
Micro-Nanostructure in Multiphase Polymer-Liquid Crystalline Materials. Susanta Kumar Das and Alejandro D. Rey; Chemical Engineering, McGill University, Montreal, Quebec, Canada.

This paper presents the computational modeling of phase separation, phase ordering, and texture formation for polymer-liquid crystal mixtures. In contrast to classical phase separations, which lead to randomly distributed microdomains of various sizes, demixing in liquid crystals leads to remarkably uniform droplets that form ordered arrays. This distinctive behavior arises from the presence of topological defects and elastic distortions around the inclusions formed during the phase separation. These forces direct the ordering of the microdomains and stabilize them against coalescence; limiting thereby the coarsening mechanism of the phase separation. We show that the ordering can be controlled on a large scale by simply controlling the macroscopic alignment of the liquid crystal. It is found that spinodal decomposition driven by liquid crystal order fluctuations can lead to colloidal crystals, where the matrix is the liquid crystalline phase and the droplets consist of the isotropic polymer phase. The driving force for crystal ordering is the local interaction between phase separation and phase ordering. The driving force for the defect network formation is the couplings between gradient orientation elasticity and mass flux. Structure and formation processes are characterized using structure factors, Fourier spectra and extent of phase separation.

AA7.8
Abstract Withdrawn

AA7.9
Understanding Micro-Mechanical Behavior in Epoxy-Alumina Composites to Enhance Fracture Toughness.
Laura M. McGrath[1,2], Joseph L. Lenhart[2], Richard S. Parnas[1] and Saskia H. King[2]; [1]Institute of Materials Science: Polymer Program, University of Connecticut, Storrs, Connecticut; [2]Materials Science and Technology Division, Sandia National Laboratories, Albuquerque, New Mexico.

Low fracture toughness limits the use of epoxy composites despite their exceptional mechanical properties and production ease. Rigid-inorganic particles incorporated in epoxy improve the fracture toughness and increase the modulus. Fundamental knowledge of the effect of filler and matrix variables on the toughening mechanisms are not fully understood. We have set out so solve this problem by developing novel epoxy composites based on four grades of alumina (Al_2O_3 with various particle size and distributions: 2, 5, 18 and 26 μm) and three different epoxies derived from bisphenol A diglycidyl ether (DGEBA) and poly(propyleneoxide) diamines of different molecular weights (Mn = 230, 400 and 2000). The Al_2O_3 reinforced epoxy was studied by dynamic torsional shear rheology and scanning electron microscopy (SEM) while the fracture toughness was quantified via the stress intensity factor (K_{Ic}). Dynamic torsional shear rheology demonstrated that T_g was not significantly affected by particle size or loading, while the storage modulus increased with Al_2O_3 volume fraction. While in most cases the addition of Al_2O_3 doubled the K_{Ic}, a larger than 6-fold increase in K_{Ic} was observed for the DGEBA-230/18μm - Al_2O_3 system at 50% loading. As expected, the incremental toughening of the epoxy decreased with increasing Al_2O_3 volume fraction. The particle sizes investigated did not effect the fracture toughness of the system. With the exception of DGEBA-230/18μm - Al_2O_3 system, an increase in fracture toughness was observed with increasing Mn of the diamine. SEM corroborates these observations and provides additional details on the micromechanical behavior at the crack tip giving support to the theory of crack-front-bowing observed for other rigid inorganic/polymer composites. These results demonstrate a promising path to a dramatic increase in fracture toughness and a better understanding of the micromechanical behavior of Al_2O_3/epoxy composites.

AA7.10
Abstract Withdrawn

AA7.11
Nanomechanics of Stimulus-Responsive End-Grafted Layers

of Poly(methacrylic acid-*g*-ethylene glycol). Miao Ye[1], Delphine Dean[2] and Christine Ortiz[1]; [1]Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; [2]Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Stimulus-responsive end-grafted polymer layers have potential use for drug delivery, cell regulation, chemical valves, and biomolecular sensors. The design and function of such polymer layers is critically dependent on a knowledge of nanoscale structure-property relationships, in particular intra- and intermolecular interactions within the polymer layer and between the polymer layer and other molecular species. In this study, the nanomechanical properties of two types of chemically end-grafted stimulus-responsive comb-type graft copolymers were studied; poly(methacrylic acid-*g*-ethylene glycol) or HS-poly(MAA-*g*-EG) with 1) M_n=27K, PEG graft density=7.7%, EG/MAA=1.90, contour length, $L_{contour}$=41 nm, and molecular separation distance, s=4.4nm and 2) M_n=15K, PEG graft density=8.8%, EG/MAA=2.20, $L_{contour}$=22 nm, s=3.9nm. Chemically specific high resolution force spectroscopy (HRFS) was carried out with probe tips (end radius$\sim$50 nm) functionalized with $HS(CH_2)_{10}COOH$ (a carboxy-terminated self-assembling monolayer or COOH-SAM) to measure the normal nanoscale interaction forces, F, as a function of probe-tip sample separation distance, D, in a series of aqueous buffer solutions of varied pH (=4-9) and constant ionic strength (IS=0.005M NaCl). The same trend in HRFS data with IS was observed for both polymer layers. On "approach" (i.e. probe tip advancing towards the polymer functionalized surface) and at high pH (=7.0), a long range, nonlinear, monotonically increasing net repulsive force was observed with decreasing separation distance with a magnitude (F<0.8nN) and range (D<30nm) that was largely independent of IS. As the pH was reduced below 7.0, the magnitude of the net interaction force dropped until switching completely to a net attractive interaction potential (pH<5 for the 27K polymer and pH<4 for the 15K polymer). This phenomenon was attributed to a conformational transition from an expanded, hydrophilic state (due to ionization of carboxylic acid groups) at high pH to a collapsed hydrophobic state at low pH (due to protonation of carboxylic acid groups causing main-chain/side-chain complexation via H-bonding and hydrophobic interactions). On "retraction" (i.e. probe tip moving away from the surface), at pH 9.0 minimal hysteresis was observed and as the pH was decreased, the amount of hysteresis increased and the curves exhibited surface adhesion. For pH $\geq$7.0, the maximum average maximum adhesion force and distance was 0.45$\pm$0.22nN and 24.1$\pm$13.8nm (27K polymer) and 0.15$\pm$0.13nN and 14.9$\pm$4.7nm (15K polymer), respectively. For pH $\leq$6.0, the average adhesion force and distance was 0.76$\pm$0.44nN and 20.0$\pm$11.8nm (27K polymer) and 1.80$\pm$0.62nN and 14.9$\pm$5.9nm (15K polymer). Ongoing theoretical modeling using Poisson-Boltzmann based polyelectrolytic electrostatic double layer theory is yielding fundamental structure-nanomechanical property relationships of these stimulus-responsive polymer layers, such as the surface charge density per unit area.

AA7.12
Effects of Composition and Process Parameters on the Mechanical Properties of Bi-Component Synthetic Polymer Fibers. Michael Sennett and Elizabeth A. Welsh; US Army RDECOM Natick Soldier Center, Natick, Massachusetts.

Recent advances in fiber spinning technology have made it possible to combine two different polymers into a single melt-spun fiber in a variety of geometries, including sheath-core, side-by-side, multi-lobe, and so-called "islands-in-the-sea." Bi-component fibers are of interest because of the potential they offer for incorporating multiple functionality into fiber and textile structures for various applications. In this study, a series of islands-in-the-sea fibers are prepared with varying polymer compositions and process conditions, and the fibers are examined to determine the effects of these variables on fiber mechanical and other properties.

AA7.13
Effect of Nanoparticle Surface Functionality on the Phase Behavior and Morphology of Block Copolymer Nanocomposites. Michelle Bowman[1], Richard Spontak[1], Jon Samseth[2,1], Keith Redmond[2,1] and Steve Smith[3,1]; [1]Materials Science & Engineering, North Carolina State University, Raleigh, North Carolina; [2]SINTEF Chemistry & Materials, Kjeller, Norway; [3]Procter & Gamble Co., Cincinnati, Ohio.

Block copolymers exhibit a wealth of morphologies that continue to find use in a diverse variety of established and emergent (nano)technologies. An intriguing and proven method by which to modify the formation of such morphologies is through the use of surfaces. While numerous studies have explored the effects of molecular confinement on such copolymers, relatively few have examined the use of nanoscale objects to controllably modify the morphological characteristics and phase behavior of microphase-ordered block copolymers via modification of internal (buried) interfaces. In this work, two poly(styrene-b-methyl methacrylate) (SM) diblock copolymers with molecular weights of $\sim$26 and $\sim$21 kDa and styrene contents of about 50 and 57 wt%, respectively, have been modified with surface-functionalized fumed silica (FS). The neat copolymers are predicted to exhibit bulk order-disorder transitions (ODTs) in the vicinity of 170 and 140 C, respectively, above which the copolymers are no longer ordered. Dynamic rheological measurements have been conducted to verify this prediction and establish a baseline for further quantitative comparison with SM/FS nanocomposites. Birefringence and small-angle x-ray scattering (SAXS) have also been performed to confirm results obtained by rheology. The surface functionalities selected here are anticipated to probe the importance of chemical interactions with the blocks of the copolymer. Unmodified FS with silanol surface groups will interact strongly with the M blocks. Similar, but less pronounced, selectivity is expected for methacrylate-functionalized FS. Another FS with octyl substitution serves as a non-selective additive within the copolymer matrix. The composition range explored extends from dilute to concentrated. Measured ODTs, as well as morphologies discerned from SAXS and transmission electron microscopy, will be presented and discussed in light of recent theoretical predictions and simulations.

AA7.14
Electrospinning of PMMA Layered Silicate Nanocomposites: Effect of Tethering Chemistry on Morphology, Dispersion Rheology and Processing. Mao Wang[1], Alex J. Hsieh[2] and G. C. Rutledge[1]; [1]Department of Chemical Engineering, Institute for Soldier Nanotechnologies, Massachusetts Institute of Technology, Cambridge, Massachusetts; [2]Army Research Laboratory, Aberdeen Proving Ground, Maryland.

Electrospinning of PMMA layered silicate nanocomposites was carried out to form fibers with diameter in the submicron range. Effects of tethering chemistry of the surfactants in contrast to clay loading levels on the morphology, dispersion rheology and fiber spinning of PMMA nanocomposites were systematically investigated. Organoclays modified with two specially designed surfactants, an alkyl ammonium surfactant with an additional reactive methacryl or styryl functioinal group, were compared with the commercial Cloisite 20A montmorillonite clay, which has two hydrogenated tallows but with no additional tethering functionality. The TEM and X-ray diffraction results reveal that exfoliation of montmorrilonite layered silicates in these in-situ polymerized PMMA nanocomposites is achieved when an additional reactive methacryl or styryl functional group is incorporated onto the alkyl ammonium surfactant. Extensional rheology measurements further point out that the presence of tethering methacryl functionality significantly increases the extensional viscosity and the longest relaxation time of the nanocomposite dispersion, favorable for electrospinning of uniform fibers. In practice, the diameter of electrospun fibers is predominated by the concentrations of the polymer matrix. This study clearly demonstrate the pathway for electrospinning of smaller diameter of fibers from polymer solutions in which the polymer matrix consists of small amount of well dispersed and exfoliated organoclay particularly with compatible tethering functionality, which otherwise are not electrospinnable at lower concentrations.

AA7.15
Micro-Compression of Nanocrystalline and Bimodal Metals. Brian Elias Schuster[1,2], Qiuming Wei[1] and K. T. Ramesh[1]; [1]Mechanical Engineering, Johns Hopkins University, Baltimore, Maryland; [2]US Army Research Lab, Aberdeen Proving Ground, Maryland.

Micro-compression is a novel technique first developed by Uchic et al. as a means to probe the compressive properties of micrometer sized compression specimen using a modification of a conventional nanoindentation system. While this has been previously applied to single crystal systems, we apply micro-compression to nanocrystalline metals, as the limited sample size makes these materials ill suited for conventional compression experiments. We further apply this technique to a bimodal (nanocrystalline and course grained) system to examine the link between micro-scale deformation and the bulk compressive properties of the material.

AA7.16
Electro-Mechanical Processes in Carbon Nanotube Materials. Hossein Golnabi[1] and Marjan Razani[2]; [1]Institute of Water and Energy, Sharif University of Technology, Tehran, Iran; [2]Institute of Water and Energy, Sharif University of technology, Tehran, Iran.

In this report a model is developed for the operation of a typical carbon nanotube actuator and the related electromechanical coupling relations and equations governing the actuation process are described. By solving such a system of equations numerically, the important

parameters such as induced strain curve are investigated. The deformation parameters for a zigzag (10,0) CNT material are investigated. As a result, the transverse dimensional is increasing with the electron charge injection level while the longitudinal dimensional charge is negative that shows a shrink in the axial direction of the CNT material. The value of the torsional deformation is constant of zero for this type of structure. The longitudinal, transverse, and torsional deformation for a chiral CNT fiber of (10,2) is presented. As shown both of the longitudinal and transverse dimensional changes are increasing with the doping percentage level while there is expansion in radial direction and there is a shrink in the axial direction of the CNT. The expansion in radial direction for this type of CNT is about 0.35% while for the axial shrink is about 0.25% for the same level of electron charging. The torsional deformation for such a CNT material is about 0.45%. At the end, possible applications of such carbon nanotube materials for the actuator and sensing devices are discussed.

AA7.17
Investigation on temperature dependence of 'G' band peak of SWNT. Massood Atashbar, Electrical and Computer Engineering, Western Michigan University, Kalamazoo, Michigan.

Since discovery of carbon nanotubes (CNTs) they have been of great interest in the field of nanoscience and technology. Carbon nanotubes exhibit unique mechanical, electrical, and thermal properties, which make them one of the most wonderful macromolecules that science has ever come across. Depending on the diameter and chirality, the nanotubes behave as conductors or moderate band gap semiconductors. Thermal stability and temperature-dependent properties of carbon nanotubes are very important for the fabrication of carbon nanotube-based devices. Raman spectroscopy is a non-destructive method to characterize carbon nanotube. Carbon nanotubes display unique and distinct Raman spectra compared to other forms of carbon due to their one-dimensional nature. They have unique structural properties due to their extremely small diameters and the curved C-C bonds. The curvature of the carbon nanotubes is responsible for some of the surprising properties like the antilocalization effect. This special feature makes single wall carbon nanotubes (SWNT) different from its planar counterparts. In this study SWNTs prepared by arc discharge process have been dissolved in chloroform and then filtered through Anatop filters with porosity of 30 nm. After sonication and deroping the bundled carbon nanotubes were then casted on silicon substrates using a micropipette. The matrix of the SWNT was studied using Atomic Force Microscope in non-contact mode. The thickness of the film was controlled by the amount and concentration of the casted solution. This study showed that at elevated temperatures the SWNT G-band peak intensity diminishes and shifts downward. This downward shift in the G band peak of CNT showed a linear trend and its temperature coefficient was found to be about 0.044cm^{-1}/K which higher is compared to the planar carbon structures (- 0.031cm^{-1}/K). A hypothesis is proposed based on structural differences in C-C bonds of the CNT and planar counterparts. SWNT can be imagined as a single sheet of graphene rolled up to form seamless cylinder. The cylinder is closed at the ends by two hemispheres of buckminster fullerene molecule. At elevated temperatures, in the planar graphite sheets, the C-C bonds elongate against the restoring force between the carbon atoms. The same restoring force does exist in the case of carbon nanotubes but a new radial component of this force arises because of the cylindrical structure of the carbon nanotube. So the restoring force now has two components one tangential and the other radial. The restoring force against the bond stretching for the SWNT is less because it is decomposed into tangential and radial component. Hence, in this case only tangential component opposes the bond stretching which results in a higher temperature coefficient. The detail of experimental results and hypothesis will be presented in the full paper.

AA7.18
Synthesis of C_{60} Polymers by Laser Irradiation under Pressure. Hiroshi Yamamoto, Ryoji Hashimoto, Shingo Ando and Nobuyuki Iwata; Electronics and Computer Science, College of Sci. & Technol., Nihon University, Funabashi, Japan.

The expected features of 3-dimensional (3D) polymers of C_{60} are appeared in extreme hardness, low density and flexibility, which might be named as a "Superdiamond". The aims of this work are to develop the synthesis process for the 3D C_{60} polymers by laser irradiation under high pressure and to study the fundamental properties of the C_{60} polymers. The anvil pressed at about 600MPa was set in a vacuum chamber which was evacuated by a turbo molecule pump. The pristine powder of C_{60} powder (99.95% purity) and/or C_{60}/I_2 mixture, in which iodine is a hole-dopant, was set in the anvil and pre-annealed at ca. 250°C for ca. 20h to remove impurities and absorbed gases. The size of samples was in a 5mm diameter and a height of less than 0.5mm. The irradiation laser was Excimer (ArF 193nm, KrF 248nm) Laser with the power of few hundreds mJ or Free Electron Laser (FEL) which has the features of tunable wavelength and high power. The fundamental wavelength of FEL was varied in the range of 1260nm-1440nm. The 3rd harmonics, 420nm-480nm were also used. The irradiation conditions were the power of few tens μJ/Pulse, the repetition cycle of 2Hz, the irradiation time of 300min. A Raman microscopic spectroscopy (Renishaw SYSTEM1000) and X-ray diffraction (XRD) (Rigaku RAD-C) were used to characterize the samples. The computer simulation of the vibration modes was done to evaluate the Raman spectrum. In the Raman spectrum of the samples irradiated and non-irradiated by FEL the vibration mode of Ag(2) show the peak at 1462.9cm^{-1} and 1459.7cm^{-1}, respectively. Furthermore the more distinct peak shift of the Ag(2) peak was observed in the case of the pristine powder of the C_{60}/I_2 mixture. The simulation revealed that the Ag(2) peak shifts to the lower energy side and/or broadens according to the polymerization of C_{60} molecules. XRD patterns showed that the distance between molecules shortened and crystallity was degraded by the laser irradiation. For example, the distances between molecules estimated from a (111) peak were shortened from 0.828nm to 0.819nm and the half-width of diffraction peaks increased by 1.5-2.0 times after the FEL irradiation. The results showed that crystalline changes toward the polymer phase took place in the samples after the laser irradiation. These results obtained suggested that the 3D polymerization of C_{60} was effectively promoted by the laser irradiation and also the hole-doping by iodine.

AA7.19
Enhanced Yield Strength and Hardness in Iron Nanocomposite with In-situ Grown Single Wall Carbon Nanotubes. Amit Goyal[1], Donald Wiegand[2], Frank Owens[2] and Zafar Iqbal[1]; [1]New Jersey Institute of Technology, Newark, New Jersey; [2]ARDEC, Picatinny, New Jersey.

The mechanical yield strength of iron-carbon nanotube composites fabricated by in-situ chemical vapor deposition of typically 2.2 volume % single wall carbon nanotubes inside an iron matrix, shows remarkable enhancement up to 45% relative to that of similarly treated pure iron reference samples without nanotubes. The flow stress, the work hardening coefficient and the Vickers hardness coefficient are also significantly increased in these composites relative to similar samples without nanotubes. X-ray diffraction in combination with energy dispersive x-ray measurements and Raman spectroscopy indicated no concomitant formation of carbides and very little amorphous carbon during the vapor deposition process. Micro-Raman spectroscopy and scanning electron microscopy showed spectral signatures and images, respectively, indicating the formation of single wall carbon nanotubes and dispersion of the nanotubes within the cavities of the iron matrix, which imply that mechanical strengthening is due to support of the cavities provided by the nanotubes.

AA7.20
Apparent Thermal Contraction of Single-Walled Carbon Nanotubes. Xi Chen and Guoxin Cao; Civil Engineering and Engineering Mechanics, Columbia University, New York, New York.

It is of fundamental value to understand the thermo-mechanical properties of carbon nanotubes. By using molecular dynamics simulation, we have carried out a systematic numerical investigation to explore the natural thermal vibration behaviors of single-walled carbon nanotubes and their implication on the apparent thermal contraction behaviors. It is found that the thermo-mechanical behavior of single-walled carbon nanotubes is exhibited through the competition between quasi-static thermal expansion and dynamic thermal vibration, while the vibration effect is more prominent and induces apparent contraction in both radial and axial directions. With increasing temperature, the anharmonic interatomic potential helps to increase the bond length, which leads to thermally induced expansion. On the other hand, the higher structural entropy and vibrational entropy of the system cause the carbon nanotube to vibrate, and the apparent length of nanotube decreases due to various vibration modes. Parallel analytical and finite element analyses are used to validate the vibration frequencies and provide helpful insights. The present study is perhaps the first systematic attempt to analyze both thermal expansion and contraction behaviors, and to obtain detailed information on various vibration modes as well as their contributions to the coefficient of thermal expansion in axial and radial directions. The study may provide useful information on the thermo-mechanical integrity of single-walled carbon nanotubes, and become important in practical applications involving finite temperature.

AA7.21
Mechanisms of Nanoindentation on Single-walled Carbon Nanotubes. Xi Chen and Guoxin Cao; Civil Engineering and Engineering Mechanics, Columbia University, New York, New York.

The mechanisms of nanoindentation on single-walled carbon nanotubes (SWCNTs) have been studied by using both molecular dynamics simulation and continuum analysis, during which a flat layer

of diamond atoms is pressed down incrementally on a vertically aligned SWCNT. SWCNTs are divided into three distinct categories based on their aspect ratios, such that the nanotube behavior transits from a shell (short tube) to a beam (long tube). Molecular dynamics simulations are used to explore the diverse indentation characteristics in each domain, where the relationships between the strain energy and indentation depth during loading, unloading, and reloading are continuously recorded. The nanoindentation mechanisms are characterized by the critical indentation depth, maximum strain energy and force associated with buckling, as well as the evolution of carbon bond length and morphology of the SWCNTs. Bifurcation behaviors are explored by investigating the loading-unloading-reloading behaviors of the nanotubes. Parallel finite element simulations are also used to study the pre- and post-buckling behaviors of SWCNT, by incorporating the Van der Waals interaction into the continuum code. It is found that for the most part continuum analysis can effectively capture the overall indentation characteristics, yet some details related to the atomic characteristics of nanoindentation may only be revealed by molecular dynamics simulation. Finally, an indentation mechanism map is derived by comparing behaviors of SWCNTs with different aspect and section ratios. Focusing on the effects of nanotube length, the multiscale study on the indentation mechanisms of carbon nanotubes may be used to determine the intrinsic mechanical properties of SWCNTs by means of nanoindentation.

AA7.22
Rate theory of yield in carbon and boron nitride nanotubes.
Traian Dumitrica[1] and Boris I. Yakobson[2]; [1]Mechanical Engineering, University of Minnesota, Minneapolis, Minnesota; [2]Mechanical Engineering and Materials Science, Rice University, Houston, Texas.

Boron nitride and carbon nanotubes have comparable mechanical stiffness. Beyond the elastic response, dislocation theory and molecular dynamics both suggest that mechanically induced defects are also similar: a 5/7/7/5 dislocation dipole emerges under strain through a Stone-Wales 900 bond flip. The same defect appears to be the lowest in energy for the corresponding carbon or boron nitride hexagonal lattices. Combining kinetic and thermodynamic arguments we obtain and compare the yield strains of these materials under different conditions (temperature, tensile-test experiment duration, nanotube sample size). For this we computed, based on density functional theory, the activation and formation energies for different bond orientations and as a function of an external strain. Once the most likely yield channel (bond orientation–rotation direction) is identified, the real time strength is determined by the rate of defect formation and decay (back-flipping to perfect lattice). Relative to carbon nanotubes, the boron nitride yield defects have lower activation but higher formation energies. This leads to an interesting phenomenon of strength crossover from these two materials under different conditions: While at moderate temperatures carbon nanotubes are stronger, at high temperatures (or extremely long times) the situation is reversed and boron nitride nanotubes are thermo-mechanically more stable. References: 1. T. Dumitrica and B.I. Yakobson, Strain-rate and temperature dependent plastic yield in carbon nanotubes from ab initio calculations, Applied Physics Letters 84, 2775 (2004). 2. T. Dumitrica and B.I. Yakobson, Rate theory of yield in boron nitride nanotubes, Physical Review B (in press).

AA7.23
Mechanical Characterization of Carbon/Metal Core/Shell Structures. Thorsten Staedler, Maik Eggers and Xin Jiang; Institute of Materials Engineering, University of Siegen, Siegen, Germany.

Structures with lateral dimensions in the nanometer regime have been objects of interest for quite a while now. Nevertheless, the direct assessment of their material properties is still afflicted with difficulties as their characteristic size causes various handling issues. Besides the electrical, magnetic, and optical behaviour, the mechanical properties of nanostructures are of special interest as these basically determine the possibility to use the structures in order to design mechanically stable devices. In this work aligned and randomly orientated carbon nanobells (CNBs) have been deposited by chemical vapour deposition (CVD) onto a silicon wafer. In a second step these structures have been electroplated with nickel, creating films of carbon/nickel core/shell structures. A series of samples with various nickel film thicknesses is available for mechanical testing. Both, individual carbon and carbon/nickel structures as well as films/networks of these structures have been mechanically characterized by scanning nanoindentation and scanning probe microscopy. The complex results, which cover the mechanical response of the system on the nano- and micro-scale, will be correlated and discussed.

AA7.24
Ultra-Smooth Nanostructured Diamond Films Grown in $H_2/He/CH_4/N_2$ Feedgas Mixtures by MPCVD.
Valery Konovalov, Andrew Melo, Shafiul Chowdhury, Shane Catledge and Yogesh Vohra; Physics, Univ. of Alabama at Birmingham, Birmingham, Alabama.

In our previous experiments, we have prepared smooth nanostructured diamond films of high hardness (∼60-65 GPa) by microwave plasma chemical vapor deposition (MPCVD) techniques using $H_2/CH_4/N_2$ feedgas mixtures [1]. Those unconventional mixtures employed CH_4 concentrations as high as 15 %, which allowed higher growth rates and better film adhesion than the more conventionally-used 1-2% CH_4 concentrations. Nanostructured diamond films with high hardness and low surface roughness were successfully deposited on Ti-6Al-4V Temporo-Mandibular Joint (TMJ) implant simulants by MPCVD. These films resulted in significant decrease in wear rates compared to uncoated samples [2]. The effect of Ar feedgas addition on the properties of CVD diamond coatings have been studied systematically [3] and resulted in formation of ultra nanocrystalline diamond films at very high Ar to H_2 ratios (90-98 % of Ar in $Ar/H_2/CH_4/N_2$ gas mixtures). Here we report the effect of He addition on the structural and mechanical properties of nanostructured ultrafine-grain diamond films deposited by MPCVD. Nanostructured diamond films were deposited on polished Ti-6Al-4V disks and TMJ simulants (having 4-5 nm RMS surface roughness) using different He/H_2feedgas ratios. The concentration of C_2 and CN plasma emission species was monitored by optical emission spectroscopy. We did not observe an increase in growth rate of diamond films grown at low He content, as reported elsewhere. Instead, the growth rate remained almost constant (at about 0.6 μm/hr) up to 80% of He. Micro-Raman spectra for films grown at all He feedgas additions show features at 1150, 1340 and 1490 cm^{-1}, typically observed for nanostructured diamond films containing sp^2 and sp^3 bonded carbon. The average grain size of diamond was estimated from the width of the (111) diamond peak in XRD spectra. An increase in He content resulted in a gradual decrease of diamond grain size from 15 nm to 9 nm. At the same time, surface roughness as measured by AFM shows a decrease from 15-18 nm to 9-10 nm. AFM images of the films show agglomeration of 20-50 nm nano-particles. Nanoindentation measurements show that the hardness and Young's modulus of the films do not decrease up to 80% of He content in the gas mixture, and were in the range of 58-72 GPa and 380-480 GPa, respectively. Measurements of wear rate and friction for these coatings and the possible growth mechanisms are discussed. These films may be used for durable wear-resistant applications such as is needed in dental and orthopedic implants. We acknowledge support from the NIH-NIDCR under Grant No. R01DE013952 and from the NSF-REU program under Grant No. DMR-0243640 (A.M.). [1] S. A. Catledge, J. Borham, Y. K. Vohra, W. R. Lacefield, and J. E. Lemons, J. Appl. Phys. 91, 5347 (2002). [2] M. J. Papo, S. A. Catledge, and Y. K. Vohra, J. Mat. Sci.-Mat. In Medicine 15, 773 (2004). [3] D. M. Gruen, Annu. Rev. Mater. Sci. 29, 211 (1999).

AA7.25
Organized defect formation in a solid. Wei Lu and David Salac; Mechanical Engineering, University of Michigan, Ann Arbor, Michigan.

Self-organized nanostructures have received increasing attention in recent years. An important class of nanostructures is regularly patterned nanovoids, which has applications from phonetic devices to biosensors. Experiments have shown that ordered nanovoids may emerge spontaneously in a solid via vacancy coalescence and diffusion. A typical example is the molybdenum system, which was first reported by Evans. Subjecting a molybdenum sample to continual irradiation of neutrons or heavy particles at elevated temperatures, vacancies emerge and agglomerate into voids. These voids form a three dimensional b.c.c lattice structure, replicating the crystal lattice of the host material. The ordered voids have diameters around 5∼7 nm and lattice spacing around 20∼30 nm. Similar phenomena have been observed in different material systems, including metals, alloys and compounds. Self-assembled defect wall structures have also been reported. Alternatively, gaseous ion irradiation, such as helium, produces self-assembled bubbles. Some general features can be identified from experimental observations. Tiny voids appear randomly in the early stage of irradiation. These voids grow and start ordering under continual irradiation at about 0.3∼0.4 melting temperature of the specimens. Then the ordering of voids expands from many early-formed small "seed" regions to other regions. There exists a threshold value of irradiation dose depending on materials, and the lattice perfection increases with the dose. However, the void ordering is insensitive to the dose rate. These observations suggest that a general mechanism may exist across different material systems. In this paper we present a dynamic model that accounts for both the elastic effect and vacancy diffusion. In particular, we highlight the surface misfit at the void/solid interface. Two significant features accompany void self-organization are phase separation and anisotropic diffusion, as revealed in experiments. Our model captures these two features. We will show that the anisotropic diffusion has close relation to the elastic anisotropy. A phase field approach is adopted. The application of a diffuse interface allows voids to emerge or dissolve

naturally, and the system can form whatever pattern it favors. A sharp interface is unsuitable for such a purpose. We incorporate the free energy of mixing, interfacial energy and elastic strain energy into the driving force for vacancy diffusion. The dynamic processes of void formation, coalescence and ordering are simulated with an efficient algorithm in Fourier Space. The simulations reveal rich dynamics. It is found that the elastic anisotropy can induce orientational preference in vacancy diffusion, even if the diffusivity is isotropic. Vacancies migrate faster along the elastic compliant directions, and cause the self-assembled voids to replicate the host crystal symmetry.

AA7.26
Fabrication of Twisted Nanofibers for Improving Mechanical Properties. B. K. Gu, S. J. Park, S. G. Yoon, M. S. Kim, M. K. Shin, I. Y. Kim, S. I. Kim and S. J. Kim; Dept. of Biomedical Engineering, Hanyang University, Seoul, South Korea.

We have developed a new method for obtaining twisted polyethylene oxide (PEO) electrospun nanofibers. The electrospinning technique is also applicable in the fabrication of various nano-scale materials, including many polymers [1], because of its simplicity and its process continuity. However, the polymer nanofibers produced by the electrospinning processes are not as strong as desired, due to the very small diameters of the resulting fibers [2]. For this reason, we modified the electric field to change the shape of the fiber in an attempt to improve the mechanical properties of our nanofibers. In this study, an electrical charge was supplied to the each side of an auxiliary polygon electrode sequentially using relay board, and twisted airborne nanofibers were obtained in a continuously rotated electric field. The charged nanofiber experienced two sets of electrostatic forces. The first electrostatic force was in the same direction as the applied electric field, and the second electrostatic force was from coulomb interactions between the airborne nanofibers and the charges on the surface of the auxiliary electrode. These electrostatic forces made it possible to transform the morphology of the fibers using the rotating auxiliary electrode relay. The twisted nanofibers were characterized using field emission scanning electron microscopy. We modeled this phenomenon by calculating the electric field strength vectors using the Maxwell finite element modeling software package. Twisted nanofibers may overcome the strength limitations of nanofibers in some applications. It is expected that this new electrospinning technique will find widespread use in the fabrication of nanofiber-based structures. References 1. Y. Dzenis, Science 2004, 304, 1917. 2. H. Hou, J. J. Ge, J. Zeng, Q. Li, D. H. Reneker, A. Greiner, S. Z. D. Cheng, Chem. Mater. 2005, 17, 967.

AA7.27
Multiscale Porous Hierarchical Structures: A Novel Approach to Modeling Their Deformation. Monica Soare and Catalin Picu; Rensselaer Polytechnic Institute, Troy, New York.

A new formulation is proposed to address the deformation of multiscale hierarchical structures with a self-similar geometry across scales for which the classical formalism either cannot be applied or it is too expensive from computational point of view. Examples of such structures are porous materials (rocks, aerogels, glasses) in which pores with a wide range of dimensions are found, many biological materials and some of the newly developed nanostructured hierarchical composites. To this end, the equations of solid mechanics are reformulated to include information about the geometry. The procedure to solve boundary value problems with the new formulation will be presented. Examples will be discussed in which the variation of the solution with the number of scales in the hierarchy is studied. The formulation allows the homogenization of such complex structures.

AA7.28
Polarized Raman Spectroscopic Study of the Deformation Behavior of Epoxy/SWNT Composites. Chih-chuan Kao and Robert J. Young; Manchester Materials Science Centre, School of Materials, The University of Manchester, Manchester, United Kingdom.

Raman spectroscopy has proved to be a powerful technique for characterizing nanotubes and determining the deformation behavior of their composites. Evidence of stress transferred from a polymeric matrix to nanotubes is the strain-induced shift of the vibrational frequency of the G' band towards lower wave numbers in tension and higher wave numbers in compression. The angular dependence of the intensity of Raman bands for nanotubes has been investigated theoretically and experimentally. These studies have demonstrated that the intensity of the radial breathing modes (RBMs), D band and G band reaches its maximum when the polarization of the incident laser is parallel to the nanotube axis. Therefore, the technique only probes the mechanical response of nanotubes that are parallel or nearly parallel to the incident laser polarization. In this study, polarized Raman spectroscopy has been utilized to investigate the angular dependence of the deformation behavior of nanotubes dispersed isotropically in an epoxy resin. The results show that the G' band shift rate depends on the configuration of the incident polarizer and analyzer. Also, the G' band shift rate varies with the angle between the incident laser and strain axis in the parallel- and cross-polarized configurations. The data was analyzed with a conventional stress theory about the angular dependence of fiber strain in a composite. The calculated Poisson's ratio (0.33) is similar to the value provided by manufacturer (0.35).

AA7.29
A High-Performance Energy Absorption System Based on Nanoporous Technologies. Yu Qiao, Falgun B. Surani and Xinguo Kong; Department of Civil Engineering, University of Akron, Akron, Ohio.

Energy absorption systems (EAS) have immense importance to automobile, aircraft, defense, construction, and manufacturing industries. They are mainly used to prevent structural damages caused by impacts, collision, and explosion, and are usually based on "soft" materials, such as reinforced polymers and shape memory alloys, that can sustain multiple-site damages or undergo dispersed phase transformations. However, currently, the energy absorption effectiveness of these materials, although already close to its limit, is still far from satisfactory. To produce high-performance protection devices, new mechanisms must be discovered. According to a recent experimental study, with appropriate porous structure and surface properties, a nanoporous material can be infiltrated by a nonwetting liquid when the pressure is sufficiently high such that the capillary effect is overcome. As the pressure is reduced, for reasons that are still under investigation, the confined liquid would remain in the nominally energetically unfavorable nanopores, and thus the excess solid-liquid interface energy can be considered as being "absorbed", leading to a significant hysteresis of absorption isotherm. Due to the ultrahigh specific surface area of the nanoporous material that usually ranges from 100-1000 m2/g, the energy absorption effectiveness of such a system can be higher than that of conventional EAS materials by orders of magnitude. By using low-molecular-weight chemical admixtures, the infiltration pressure can be adjusted in a broad range from 0 to about 20 MPa, and the system recoverability can be improved to 70-80%, that is, the system can be used repeatedly. A thermodynamic model has been developed to capture the confinement effect of pore walls and the mass/energy exchange between liquid/gas phases in nanoenvironments.

AA7.30
Structure and Properties of Electrospun PLLA Single Nanofibers. Ryuji Inai[1], Masaya Kotaki[2] and Seeram Ramakrishna[1,3,4]; [1]Department of Mechanical Engineering, National University of Singapore, Singapore, Singapore; [2]Molecular & Performance Materials Cluster, Institute of Materials Research & Engineering, Singapore, Singapore; [3]NUS Nanoscience and Nanotechnology Initiative, National University of Singapore, Singapore, Singapore; [4]Division of Bioengineering, National University of Singapore, Singapore, Singapore.

Polymer nanofibers have been attractive materials for a wide range of applications because of their large surface area to volume ratio and the unique nanometer scale architecture built by them. Their potential applications are tissue engineering scaffolds, drug delivery media, filtration media, protecting clothes, and many more. It is well known that the properties and internal molecular structure of polymer solids are greatly affected by the processing conditions. Therefore, an understanding of the processing-structure-property relationship is essential for engineering polymer nanofibers to meet the demands of applications. Electrospinning is a superior method for producing continuous nanofibers from most polymers. Due to the particular interests of electrospun nanofibers in tissue engineering fields, great efforts have been made to study the effects of processing parameters (solution properties, processing conditions, ambient conditions) on the morphology of electrospun biodegradable polymer fibers. The individual parameters have been well analysed in each polymer; however, no comprehensive study has yet been completed. Due to limitations of characterization methods, structure-property relationship of electrospun polymer fibers has not been clarified yet. In our previous studies, systematic parameter studies was conducted and ultra-fine nanometer scale PLLA fiber with a 9nm fiber diameter was successfully electrospun. In the study, the solution conductivity and polymer concentration were indicated to have an important role in controlling the fiber diameter. Decreased fiber diameter might be due to large elongation of a fluid jet during electrospinning. The elongation process may affect the internal molecular structure transformation in electrospun fibers, but it has not been reported yet. Another possible parameter which may affect the internal molecular structure is the take-up velocity, as many researchers have investigated in melt-spinning. In this study, semi-crystalline poly(L-lactide) (PLLA) were electrospun into nanofibers. Processing parameter (solution conductivity, polymer concentration, take-up

velocity) effects on the internal molecular structure of electrospun PLLA nanofibers were investigated by x-ray diffraction (XRD) and differential scanning calorimetry (DSC). Take-up velocity was found as a dominant parameter to induce a highly ordered molecular structure in the electrospun PLLA fibers compared to solution conductivity and polymer concentration, although these two parameters have been known to play an important role in controlling the fiber diameter. A collecting method of a single nanofiber by an electrospinning process was developed for the tensile tests to investigate structure-property relationships of the polymer nanofibers. The tensile results indicated that higher take-up velocity caused higher tensile modulus and strength due to the ordered structure developed through the process.

AA7.31
SiC Nanofiber Synthesis and Potential Applications in Ceramic Composite Coatings. Abhishek Kumar Kothari[1], Hao Li[2] and Brian W. Sheldon[1]; [1]Engineering, Brown University, Providence, Rhode Island; [2]Department of Mechanical & Aerospace Engineering, University of Missouri-Columbia, Columbia, Missouri.

SiC nanofibers were synthesized by reacting multiwalled carbon nanotubes with Si-containing vapor. A mixture of Si and SiO2 powder was used to generate these vapors. High resolution TEM and XRD analysis confirmed that the resulting materials have a βSiC structure. A model of the conversion process was developed from the TEM results, and from detailed thermochemical and mass transport analyses. The experimental and modeling results demonstrate that the conversion process is highly sensitive to both the temperature and the gas composition. Ceramic matrices around the SiC nanofibers were fabricated with chemical vapor infiltration. Nanoindentation was used to investigate the basic mechanical properties of these composite materials. These properties were also compared with analogous composite coatings that were fabricated with carbon nanotubes.

AA7.32
Crack Resistance in Silicon Carbide: An Atomic Scale Investigation. Alessandro Mattoni[1], Luciano Colombo[1] and Fabrizio Cleri[2]; [1]SLACS Sardinian Laboratory for Computational Materials Science, Monserrato (Ca), Italy; [2]ENEA, Unita Materiali e Nuove Tecnologie, Roma, Italy.

By means of atomic-scale simulations we investigate the physical meaning of the intrinsic crack resistance in the Griffith theory of brittle fracture. Atomistic simulations offer the opportunity to study the fundamental issues underlying the Griffith theory in ideally pure, perfect single-crystal materials under uniaxial load. We focus our work on the silicon carbide since it is the prototype of an ideally brittle material up to extreme values of strain rate and temperature and because of its technological relevance as a structural and nuclear material. Atomic forces were calculated according to the Tersoff model that is able to describe the mechanical brittle behavior of cubic β-SiC and has been applied to investigate the static mechanical response of nanostructured β-SiC to uniaxial tensile loading.[1] By simulating systems containing up to 250,000 atoms we address the relationship among the critical load to fracture, intrinsic crack resistance and surface energy, in the framework of Griffith theory.[2] We find that the widely accepted identification of intrinsic crack resistance with the cleavage surface energy actually underestimates the energy release rate. It is also proved that a large part of such a discrepancy can be attributed to the strain dependence of the Young modulus and surface energy. Moreover, we set an upper bound for the role of lattice trapping in increasing the effective crack resistance. Finally, for the shortest microcracks we find that crack resistance can be fitted by an empirical elasto-plastic model. [1]A. Mattoni, L. Colombo, and F. Cleri, Phys. Rev. B 70, 094108 (2004). [2]A. Mattoni, L. Colombo, and F. Cleri, submitted for publication (2005).

AA7.33
Atomic-Scale Analysis of Ductile Void Growth and Nanocrystalline Domain Formation as Strain Relaxation Mechanisms in Ultra-Thin Metallic Films. M. Rauf Gungor and Dimitrios Maroudas; Department of Chemical Engineering, University of Massachusetts, Amherst, Massachusetts.

As the feature size of electromechanical devices shrinks toward the nanometer scale, understanding the atomistic mechanisms of strain relaxation becomes essential for improving materials reliability in microelectronics and advancing nanofabrication techniques. Atomic-scale modeling based on molecular-dynamics (MD) simulations provides a powerful means for analyzing strain relaxation mechanisms in metallic thin films and enables the development of constitutive relationships for continuum modeling of metallic thin-film mechanical behavior. In this presentation, we report a systematic computational analysis of the atomistic mechanisms of strain relaxation over a wide range (up to 17%) of applied biaxial tensile strain in free-standing ultra-thin Cu films with and without cylindrical voids extending throughout the film thickness. The analysis is based on isothermal-isostrain MD simulations within an embedded-atom-method (EAM) parameterization for Cu and using slab supercells that contain millions of atoms. Our analysis has revealed various regimes in the film's mechanical response as the applied biaxial strain level increases. After an elastic response at low strain ($< 2\%$), plastic deformation occurs accompanied by dislocation emission from the void surface and propagation of threading dislocation loops initiating at the film surface. Over the strain range following the elastic-to-plastic deformation transition ($< 8\%$), ductile void growth is the major strain relaxation mechanism through the radial expansion of a plastic zone that surrounds the void. At higher levels of applied strain ($> 8\%$), a subsequent transition to a new strain relaxation regime gives rise to a practically uniform distribution of dislocations in the metallic thin film. Under such conditions, formation of nanometer-scale domains of fcc crystalline material mediates the transformation of the initially single-crystalline metallic film to a nanocrystalline structure. Furthermore, void growth is inhibited as the dislocations emitted from the void surface are pinned by their interaction with the simultaneously generated network of defects in the nanocrystalline material. By comparing MD simulation results in identical thin films with and without voids, it is also demonstrated that strain relaxation at high levels of strain ($\geq 12\%$) is not affected by a pre-existing void in the metallic film.

AA7.34
Structural Transformation of Nanobelts under Stress. Helin Wei, Jian Wang and Hanchen Huang; Department of Machenical, Arospace, and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, New York.

Nanostructures are the backbone of nanotechnology. Because of large surface-to-volume ratio, nanostructures such as nanowires and nanobelts undergo structural transformations from surface sites. Using molecular dynamics simulations, we show that structure transformations occur in face-centered-cubic (FCC) metallic nanobelts, under a combination of intrinsic and extrinsic stresses. First, a nanobelt with {100} surfaces transforms to another nanobelt of {111} surfaces through dislocation nucleation at surfaces. Second, it is the combination of intrinsic and extrinsic stresses that trigger the transformation. For 5d metals such as Au, the intrinsic surface stress is large and the necessary extrinsic stress is small. In contrast, the intrinsic surface stress is small and therefore the necessary extrinsic stress for the transformation is large. The simulation results are relevant to technologies involving nanobelts under mechanical loading.

AA7.35
Fracture Behavior of Nanoporous Organic Thin-Films. Andrew V. Kearney[1], Carol E. Mohler[2], Michael E. Mills[2] and Reinhold H. Dauskardt[1]; [1]Materials Science and Engineering, Stanford University, Palo Alto, California; [2]Advanced Electronics Materials, The Dow Chemical Company, Midland, Michigan.

Nanoporous layers are being considered for a range of applications, including interlayer dielectrics in microelectronics to biosensors and size-selective membranes for biotechnologies. In all cases, their mechanical and fracture properties are of critical importance for reliable integration. In the present study involving poly(arylene) ether (PAE) polymer films, we present surprising evidence that nanoporous forms of these films exhibit increasing fracture energy with increasing porosity. Such behavior is in stark contrast to a wide range of reported behavior for porous solids, which indicates that the fracture toughness typically decreases markedly with increasing porosity. A ductile nano-void growth and coalescence fracture mechanics-based model is presented to rationalize the increase in fracture toughness of the voided polymer film. The model is shown to explain the behavior in terms of a specific scaling of the size of the pores with pore volume fraction. It is demonstrated that the pore size must increase with close to a linear dependence on the volume fraction in order to increase rather than decrease the fracture energy. Independent characterization of the pore size as a function of volume fraction is shown to confirm predictions made by the model. Implications for the optimum void size and volume fraction are considered for superior fracture resistance of the nanoporous films.

AA7.36
Dislocation Core Radii in Carbon Nanotubes: Continuum and Atomistic Analysis. Elif Ertekin[1,2] and Daryl C. Chrzan[1,2]; [1]Materials Science and Engineering, University of California, Berkeley, Berkeley, California; [2]Materials Sciences Division, Lawrence Berkeley National Laboratories, Berkeley, California.

In carbon nanotubes, the Stone-Wales defect plays the role of a dislocation dipole in a typical bulk system. Like their three-dimensional counterparts, these dipoles can arise from lattice distortions due to externally applied strains, dissociate, and migrate through the nanotube lattice in a process that is often likened to plastic deformation in the bulk. Thanks to the two dimensional nature

of the system, it is possible to more readily explore this behavior both atomistically and via continuum descriptions. Via ab initio descriptions, molecular dynamics, and continuum analysis, we show that dislocations in carbon nanotubes have long range stress fields whose interactions are non-negligible. The combined atomistic/continuum approach allows us to extract the core radius of the dislocation in the nanotube. This in turn provides a simple and transferrable approach to (1) determining the formation energy of a Stone-Wales defect in any carbon nanotube, and (2) exploring the dissociation and migration of the constituent dislocations. Using the core radius/continuum approach, it will likely be possible to develop plasticity models of dislocation flow in carbon nanotubes.

AA7.37
On Deformation of Metallic FCC Nanoparticles. Victor Tsai, Lew Rabenberg and Paulo J. Ferreira; Materials Science and Engineering Program, University of Texas at Austin, Austin, Texas.

Nanocrystalline FCC materials show excellent material properties, including high hardness and high yield stress. Classically, one would expect such an increase in hardness and yield strength for smaller grain sizes according to the empirical Hall-Petch equation. However, at a critical nanoscale grain size, this mechanism seems to breaks down. Despite the number of interesting papers published on this topic, controversy continues to exist. Recently, a new deformation mechanism has been observed in nanocrystalline aluminum, raising even further controversy. Molecular dynamic simulations and high-resolution transmission electron microscopy show that nanocrystalline aluminum deforms by mechanical twinning. Yet these results are surprising: as Al has a high stacking-fault energy, the presence of partial dislocations are expected to be unstable. The purpose of this paper is to offer a plausible explanation for the occurrence of faults and deformation twins in nanocrystalline Al. A simple model is developed for the nucleation and growth of both perfect and partial dislocations loops in single-crystal nanoparticles of Al with different sizes. The model shows that as the size of the nanoparticles decreases, partial dislocations are more likely to occur. Moreover, for a constant applied stress, there is a critical size at which a higher probability for the nucleation of partial dislocations occurs, compared to that of perfect dislocations. For example, for an applied stress of 1.3 GPa, the nucleation of partial dislocations becomes favorable for nanoparticles with sizes below 7 nm.

AA7.38
Mechanical Properties of Free-Standing Nanoporous Gold Nanowires. Dongyun Lee and Jeffrey William Kysar; Mechanical Engineering, Columbia University, New York, New York.

The mechanical properties of free-standing nanowires consisting of nanoporous gold are studied experimentally. The nanoporous gold is synthesized from "white gold" leaf (50% Au and 50% Ag) with an approximate thickness of 100 nm to 150 nm which is attached to a silicon substrate. The in-plane grain size of the leaf as investigated with Electron Backscatter Diffraction (EBSD) is of the order of tens of microns. Specimens suitable for mechanical testing are fabricated within individual grains of the leaf via standard lithographic techniques. The final specimen is in the form of a "dog bone". The ends of the specimen are anchored to the silicon substrate and the silicon below the gauge section is etched away, which results in a free-standing gauge section. The gauge length of the specimen is eight micrometers and the cross-sectional dimensions of the gauge length are about 150 nm by 250 nm. The specimen is then dealloyed using nitric acid, which etches away the silver and leaves open-pored nanoporous gold. The sizes of the ligaments and the voids are of the order of tens of nanometers and can be tuned with processing parameters. Importantly, the residual stress in the specimen is negligible. The mechanical properties of the nanoporous gold are probed by deflecting the gauge section with a nanoindenter. Preliminary results suggest that material deforms elastically up to a stress of 400 MPa, after which failure occurs in what is apparently a brittle manner, although it may be accompanied by plastic deformation in some of the ligaments.

AA7.39
Mechanical Strength of Semiconductor Nanowires by Atomistic simulation. Keonwook Kang and Wei Cai; Mechanical Dept., Stanford Univ., Stanford, California.

Using the atomistic simulation of the tension test with Tersoff and Stillinger-Weber potentials, we study the mechanical strength of silicon and germanium nanowires of 5nm diameter. By controlling the strain along the [110] growth direction and calculating the corresponding Virial stress until the nanowire breaks, we obtain the stress and strain curve, Young's modulus and the critical strength for nanowires's breakage. To stimulate the breaking process, a screw dislocation is intentionally introduced into the nanowire such that the system has (111) slip plane and [10-1] Burgers vector to acquire the maximum Schmid factor. Through this work, we observe the silicon and germanium nanowire are broken by shear on (111) plane. The authors build an analysis model to confirm the breaking pattern of nanowires by comparing the theoretical tensile and shear strength of bulk silicon and germanium.

SESSION AA8: Nanoindentation and Testing
Chair: A. Ngan
Thursday Morning, December 1, 2005
Republic B (Sheraton)

8:00 AM AA8.1
Grain Size Effect on the Nanomechanical Properties and Deformation Behavior of Copper under Nanoindentation Test. Shou-Yi Chang, Ting-Kui Chang and Yu-Shuien Lee; Department of Materials Engineering, National Chung Hsing University, Taichung, Taiwan.

The strengths of materials have been reported to increase with decreasing grain size as the well known "Hall-Petch effect". When the grain sizes are smaller than 15 nm, the strengths are expected to decrease with decreasing grain size, and the deformation behavior will change to grain boundary sliding or grain rotation, instead of dislocation activity. However, these results are generally proposed based on molecular dynamics simulation, and few experimental measurements are provided. Therefore in this research, the mechanical properties and deformation behavior of copper with different grain sizes have been experimentally investigated using instrumental nanoindentation. As received and thermally annealed bulk copper, and sputtered, electroplated and electrolessly deposited copper films with different ranges of grain size were used for the measurement. The hardness was found to increase, from 1.2 GPa for the bulk copper specimens with a very large grain size up to 200 μm, to about 2.3 GPa for the electroplated copper films with a grain size of several tens of nanometers. Then the harness of electrolessly deposited copper films with a grain size of only several nanometers dropped to 1.5 GPa due to the so-called "reverse Hall-Petch effect". However, the elastic constants of these copper specimens were all measured around 120-140 GPa, indicating the valid measurement of the intrinsic property. Moreover, other nanoindentating mechanical responses of the copper specimens, like true stress, deformation behavior and fracture energy release rate, were also analyzed. From the converted true stress-depth curve, it was clearly observed that the Cu specimens deformed elastically at first and then yielded at indentation depths of about 5-10 nm. The critical stresses for the initiation of plastic deformation in the copper specimens with grain sizes larger than 15 nm were measured as about 9-11 GPa, close to the theoretical stress for the shear yielding of copper. However, the critical stress for the plastic initiation of electrolessly deposited copper films with a grain size smaller than 15 nm was measured as only about 3.5 GPa due to their different deformation mechanism by grain-boundary sliding or grain rotation rather than dislocation formation and sliding. Moreover, the creep behavior of the copper specimens was also investigated by using nanoindentation test. The creep strain-stress relationship exhibited a typical power law expression. The copper specimens with smaller grain sizes showed larger creep strain rates but lower stress exponents than other specimens with larger grain sizes, implying the fast but fixed diffusion paths and grain-boundary sliding through the larger amounts of grain boundary.

8:15 AM AA8.2
Initiation and Slip Propagation During Indentation in FCC Alloys. David F. Bahr[1], Kevin A. Nibur[1], Gus Vasquez[1,2], Ali Zbib[1], Firas Akasheh[1] and Hussein Zbib[1]; [1]Mechanical and Materials Engineering, Washington State University, Pullman, Washington; [2]Los Alamos National Laboratory, Los Alamos, New Mexico.

Nanoindentation testing allows testing of both the onset of plasticity as well as the propagation of dislocations. By coupling nanoindentation, atomic force microscopy, and orientation imaging microscopy with computational simulations it is possible to gain a better understanding of the fundamental properties which can be determined on engineering alloys and model single crystals systems using localized hardness testing. Recent work has demonstrated the ability to quantify the stress required to nucleate dislocations in dislocation free solids. These observations are only possible using small scale mechanical testing, large volume mechanical testing will generally measure the motion of pre-existing dislocations under applied stresses. The effects of solute impurities in the copper-nickel system on the onset of plasticity in a previously dislocation free region have been demonstrated to be minimal. The shear stress required to nucleate dislocations in copper is approximately 1.6 GPa, while in nickel a 3.9 GPa shear stress is required. Changes in shear stress for nucleation track closely with changes in elastic modulus, showing the nucleation stress is approximately 1/30 to 1/20 of the shear modulus.

Similar behavior is demonstrated in a complex austenitic stainless steel alloy with hydrogen charging; the onset of plasticity correlates very well to changes in elastic modulus due to solute hydrogen and occurs at 1/18 of the shear modulus. Pre-existing dislocations in tungsten are shown to impact the yield point phenomena during nanoindentation, and a volumetric scaling relation between dislocation density and the shear stress at which the yield point occurs is described. Experiments will be presented at which a maximum shear stress of 1.2 GPa can be applied to a sample with a dislocation density of 1.8 etch pits per square micron (in a region around a larger indentation so that there is a gradient of dislocation density). After a discussion of the onset of plasticity, the propagation of dislocations around nanoindentation and their resultant emergence at the free surface in FCC alloys will be examined for determining the effects of tip shape, effective strain, and crystallography on the slip patterns around indentations. These patterns are compared to results from discreet dislocation dynamics simulations, and are shown to correlate well with the resolved shear stress at the elastic - plastic boundary. The saturation of slip steps on the surface is demonstrated through a series of reloading experiments in a given indentation, and it will be unambiguously shown that individual steps are only active while near the elastic - plastic boundary.

8:30 AM *AA8.3
Temperature and Rate Dependence of Incipient Plasticity During Nanoindentation. Christopher A. Schuh, Jeremy K. Mason and Alan C. Lund; Materials Science and Engineering, MIT, Cambridge, Massachusetts.

For nanoindentation of clean crystalline surfaces, the onset of plasticity is associated with a discrete displacement burst event that is widely believed to correlate with the nucleation of dislocations. Here the time- and temperature-dependencies of this phenomenon are explored for single crystals of platinum, employing a unique capability in high-temperature nanoindentation. For indentation loading rates spanning three orders of magnitude and temperatures ranging from 25 to 200 degrees C, incipient plasticity is shown to exhibit the characteristics of thermal activation. A statistical framework is presented to analyze the data and extract the activation parameters; these point to an atomic-scale process as the rate-limiting step in plastic yield at the nanoscale.

9:00 AM AA8.4
Volume and Time Dependence, and Statistical Scatter of Initial Yield Strength of Small Crystals. Alfonso H. W. Ngan, P. C. Wo and Le Zuo; Mechanical Engineering, University of Hong Kong, Hong Kong, Hong Kong.

The current rapid advancement in the nano- and micro-technology pushes for a fundamental understanding of the materials properties in the sub-micron length scale. Recent compression experiments on micro-pillars revealed that their initial yield strength increases significantly as the sample size decreases. During nanoindentation on annealed crystals, the critical load for incipient plasticity to occur is not a constant at a fixed temperature, but is found to exhibit significant statistical scatter on repeated testing. Under prolonged holding of the indentation load in the elastic regime, yielding may eventually take place after some waiting time, which is not a constant but also exhibits significant stochastic scatter. During nano-scratching under a constant normal load initially in the elastic regime, the scratch may develop into plastic deformation at some point, the location of which is also stochastic. The above statistical aspects as well as the size and time dependence of yielding in the micron-to-submicron regime resemble the characteristics of the fracture strength of bulk ceramics, which are well-known to be describable by a survival probability concept within the Weibull statistics. In the present work, a similar theoretical framework is proposed, but unlike the Weibull statistics for bulk ceramics which are empirical, the present treatment on the initial yielding of submicron crystals is based on direct observations from molecular dynamics simulations of the incipient plastic process in highly sheared Ni_3Al. From the distribution function of the interatomic displacements observed in the MD simulations, the probability of a general material volume to survive under a general condition is predicted. The survival probability is then calculated for several situations, including homogeneous deformation and nanoindentation, to predict the critical load for incipient plasticity to occur in these situations. The predicted results are found to compare favorably with the experimental results on Ni_3Al described above.

9:15 AM AA8.5
The Relationship Between the Strain Rate Sensitivity of the Flow Stress and the Strain Rate Sensitivity of The Hardness in Nanoindentation Creep. Abdelmageed A. Elmustafa[1,3], Sadi Kose[2], Winston O. Soboyejo[3] and Donald S. Stone[4]; [1]Mechanical Engineering, Old Dominion University, Norfolk, Virginia; [2]Civil and Environmental Engineering, University of Wisconsin-Madison, Madison, Wisconsin; [3]Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey; [4]Materials Science and Engineering, University of Wisconsin-Madison, Madison, Wisconsin.

This paper establishes the relationship between the strain rate sensitivity of the hardness ν_H=dlnH—/—dln$\dot{\epsilon}_H$, where $\dot{\epsilon}_H$ is an effective strain rate in the plastic zone beneath the indenter, and the strain sensitivity of the flow stress ν_σ , where ν_σ is measured using a conventional (uniaxial) experiment. We use finite element analysis to simulate nanoindentation creep to derive this relationship. The data obtained from the simulations are analysed the way they would be if they were real experimental data. We find that the ratio ν_H/ν_σdepends on the ratio of hardness (H) to Young's modulus (E), but otherwise is relatively insensitive to ν_σ as well as work hardening properties of the material. Materials with low H/E exhibit little or no difference between ν_H and ν_σ; however, as the ratio H/E increases, the ratioν_H/ν_σ decreases. The trend of the data generated from finite element analysis can be explained based on the relationship H=k$\times\sigma$ in which K depends on the ratio σ/E. The calculation of the activation volume from nanoindentation hardness experiments requires correcting for the difference in the ratio of the rate sensitivity of the hardness to the rate sensitivity of the flow stress.

9:30 AM AA8.6
Quantitative TEM of Deformation under Low-Load Indents. Kirsten K. McLaughlin, Stephen J. Lloyd and William J. Clegg; Materials Science and Metallurgy, University of Cambridge, Cambridge, United Kingdom.

Rotation of the crystal lattice under low-load indents has been identified in a variety of materials (1-3), including copper and spinel. In soft materials, these rotations are attributed to geometrically necessary dislocations arising from the strain gradients under the indenter (4,5). Experimental confirmation of these theories is difficult, as the dislocation densities under the indenter are so high that single dislocations cannot be identified in the transmission electron microscope (TEM). To identify the extent that geometrically necessary dislocations contribute to the deformation under an indenter, local crystal orientations and lattice parameters were measured using convergent beam electron diffraction (CBED) in two single crystal materials. A Knoop indenter tip was used to make low-load indents (25 to 100 mN) in a soft fcc metal, copper, and a hard cubic ceramic, spinel. The crystals were cut perpendicular to the long axis of the indent and thinned using a focussed ion beam workstation so that the deformed region under the indent could be studied in the TEM. The CBED patterns were generated from areas of less than 75 nm^2 in a foil about 200 nm thick in the direction of the electron beam. The orientation of the local crystal lattice under the convergent beam was measured from the Kikuchi lines at low camera lengths and mapped across the plastic zone. Using the relative positions of deficiency lines from the higher order Laue zone, the local lattice parameters were measured to calculate the residual elastic strain in the crystal lattice. The use of both of these techniques allows the elastic strains and rotations to be mapped in the area around the indentation. For instance, rotations from an indent to a depth of 500 nm in copper produced rotations as high as 7.7 °, while a 300 nm indent in spinel produced rotations of 8 °. Differences in indentation behaviour between the two materials can be identified through the rotation patterns. [1] N.A. Stelmashenko, M.G. Walls, L.M. Brown and Yu. V. Milman. Acta metall. mater. 41 (10), 2855 (1993). [2] S.J. Lloyd, A. Catellero, F. Giuliani, Y. Long, K.K. McLaughlin, J.M. Molina-Aldareguia, N.A. Stelmashenko, L.J. Vandeperre and W.J. Clegg. Proc. Roy. Soc. A. In press. [3] W. Yang, B.C. Larson, G.M. Pharr, G.E. Ice, J.D. Budai, J.Z. Tischler and W. Liu. J. Mater. Res. 19 (1), 66 (2004). [4] J.F. Nye. Acta metall. 1, 153 (1953). [5] H. Gao, Y. Huang, W.D. Nix and J.W. Hutchinson. J. Mech. Phys. Solids 47, 1239 (1999).

10:15 AM AA8.7
Beyond Hardness: Characterization of Rapidly Quenched Small Volume Structures using Nano-indentation. Andrew Gouldstone, Meng Qu and Jae H Kim; Materials Science and Engineering, Stony Brook University, Stony Brook, New York.

The thermal spray (TS) process produces meso-scale materials composed of an assemblage of rapidly-quenched, impacted, small-volume (micron-thickness) structures ('splats'). Knowledge of the mechanical behavior of these splats and their interaction is critical to the prime-reliant design of TS materials, Beyond this, splats represent a fascinating class of materials exhibiting ultra-fine columnar grain structure, nano-crystalline 'chill zones', residual stresses and, under certain conditions, surface oxidation, all of which affect inelastic deformation. Nano-indentation is well-suited for the characterization of splats; previous efforts have illustrated the ability to probe single-splat-on-substrate behavior (hardness, reduced modulus) using this method. What remains to be accomplished is the creative expansion of indentation techniques to explore other aspects

of splat behavior, including e.g., anisotropy and adhesion. In this talk, we present results of indentation on metallic splats, to probe the above characteristics, and to investigate behavior after heat treatment and large deformation. In addition, we discuss differences between indentation of single splats on substrates and those within assemblages, and effects of local conditions on modulus extraction. Finally, we present methods to compare nano-indentation response to in-plane behavior. Acknowledgments: Support provided by NSF CAREER award: CMS-0449268

10:30 AM AA8.8
Atomic-scale Simulations of Localization During Nanoindentation of Metallic Glasses. Yunfeng Shi and Michael L. Falk; Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan.

Nano-indentation studies provide a unique tool for understanding the mechanisms of nano-scale plasticity. We have performed molecular dynamics simulations of the nano-indentation process in model bulk metallic glasses (BMGs). Both two-dimensional [1] and three-dimensional models [2] have been simulated. In agreement with experiment these simulations reveal dramatic localization beneath the indenter. Simulation studies also clearly indicate that the quench history of the glass can play a critical role in affecting the degree of localization. By analyzing the atomic structure of the materials we note that the localization process causes a breakdown of quasi-crystal-like short-range order. We also observe that discontinuities of the load-displacement curve correlate closely with the nucleation of shear bands and the propagation of shear band slip. [1] Applied Physics Letters, Vol. 86, pp. 011914 (2005) [2] Scripta Materialia, 2005, in press.

10:45 AM AA8.9
Nanomechanical Characterization of c and a Domains in Tetragonal Barium Titanate. Xiaodong Li[1], Young-Bae Park[2], Zhi-Hui Xu[1], Matthew J. Dicken[2] and Harry A. Atwater[2]; [1]Department of Mechanical Engineering, University of South Carolina, Columbia, South Carolina; [2]Thomas J. Watson Laboratory of Applied Physics, California Institute of Technology, Pasadena, California.

The domain switching and phase transition (symmetry change) in ferroelectric thin film materials can induce local strain (stress) and hence change mechanical properties. Nanoindentation is a useful technique to measure the mechanical properties of solid surfaces and thin films, such as elastic modulus, hardness, and fracture toughness at a very local level. In this study, nanomechanical properties of c and a domains in tetragonal barium titanate were measured by nanoindentation techniques. The domain switching during indentation was studied by piezo force microscopy. The indentation stress-strain fields were obtained by finite element analysis. The domain switching mechanisms are discussed in conjunction with the lattice structure of c and a domains, indentation stress-strain fields, and mechanical properties.

11:00 AM AA8.10
New Device for Stable Mechanical Characterizations of Free Standing Films. Shakti Chauhan, Hui Wang and Ashraf Bastawros; Aerospace Engineering, Iowa State University, Ames, Iowa.

A new testing methodology is devised to test free standing films in a stable manner. The device utilizes compliant mechanisms which arrests deformation instabilities and premature failure. The device design and performance has been calibrated with finite simulation and verified experimentally. The tensile and fracture toughness of annealed and cold rolled copper films with thicknesses in the range of 10-100micron have been tested. For the annealed film, excessive ductility has been observed at strains in excess of 20-30%. The yield strength and hardening characteristics have shown both size dependent as well as size independent response. The observed trend has a strong correlation with the number of the grains within the film thickness rather than the gage thickness itself. Details of the deformation mechanisms at the grain level have been observed by digital image correlations. The deformation maps showed the evolution of the heterogeneous deformation within the film gage section into localized deformation bands having characteristic length scale of several grain sizes.

11:15 AM AA8.11
Method for Determination of Elastic Coefficients for Individual Nanostructures Based on a Technique Using the Detection of an Harmonically Modulated Charge.
Razvan Ciocan, Jay Gaillard, Malcolm J. Skove and Apparao Rao; Physics and Astronomy, Clemson University, Clemson, South Carolina.

The method used in this study is based on electric detection of charge distributed at the end of an individual nanostructure. The charge is generated by applying an AC voltage with tunable frequency. An individual nanostructure (MultiWall NanoTube -MWNT - or a NanoSpring-NS) was placed on a very sharp tungsten tip. The counter electrode consisting of a gold-coated tungsten tip was brought in close proximity and aligned with the nanostructure to be investigated. The relative position of the two electrodes was carefully monitored using a dark field microscope instrumented with a digital camera. By tuning the frequency of the ac signal, the charge on the cantilevered nanostructure can be excited in such a way that a maximum in amplitude of the charge and in the change of phase are achieved simultaneously when the frequency of the drive signal matches the mechanical resonance frequency of the nanostructure. All measurements reported in this study were performed in air under ambient conditions using a lock-in amplifier at the second harmonic. The system shows a high quality factor for ambient conditions (Q = 36). A computerized data acquisition system for acquiring the amplitude and phase provided by an oscillating individual nanostructure as a function of excitation frequency was developed for this study. For an MWNT (characterized by length L =10 μm, outer diameter D_o = 57 nm and inner diameter D_i = 17nm) the first three modes of oscillation were identified by monitoring the amplitude and phase changes. The corresponding frequencies determined experimentally were: f_{1e}= 0.339 MHz, f_{2e}= 2.42 MHz and f_{3e}= 5.31 MHz. Based on all these three frequencies, value of Young's modulus, E_b, was determined using an iterative algorithm that mainly computes the series of frequiencies based on updated values for E_b. The value thus obtained for Young's modulus is E_b = 0.0296 TPa. This value is in excellent agreement with values reported in literature for nominal E values [1] and ranging from 18 GPa to 68 GPa. The authors of the cited study measured the tensile strength of individual MWNT using a direct method: stress-strain curves were generated using a "nanostressing stage" in a scanning electron microscope. A nanospring was excited with an electrical force that acted longitudinally (along the axis of the nanospring) corresponding to the pure axial tensile load case. In this case the shear modulus, G, was calculated directly from resonance frequency. For a nanospring (with outer diameter 239 nm and pitch 178 nm) the fundamental natural frequency was determined to be 9.3MHz. The shear modulus, G, was calculated to be $\sim$2.56 GPa, a value in good agreement with one previously reported in literature, G $\sim$ 2.5 GP [2], obtained using a direct method. 1. M.Yu, O. Lourie, M. J. Dyer, K. Moloni,T. F. Kelly, R. S. Ruoff, Science, Vol 287, pp637, 2000. 2. X. Chen, S. Zhang, D. A. Dikin, W. Ding, R. S. Ruoff, Nanoletters , Vol.3, No. 9, 1299-1304, 2003.

11:30 AM AA8.12
Mechanical Testing of Freestanding Nano-Films Using a Novel Finite Diameter Tip MEMS-based Testing Machine.
Zayd Chad Leseman[1], Thomas Mackin[1] and Matthew Begley[2]; [1]Mechanical Engineering, University of Illinois Urbana-Champaign, Urbana, Illinois; [2]Materials Science and Engineering, University of Virginia, Charlottesville, Virginia.

We present a new experimental method for measuring the mechanical properties of nanoscale-thick materials using the free-standing membrane test. Freestanding circular membranes are centrally deflected using a spherical indenter attached to a microfabricated fixed-fixed beam device. Experiments of this type allow us to extract mechanical properties of the thin films without the complicating effects of the substrate, enabling accurate study of length scale effects. These experiments differ from previous work by testing freestanding films and by including the finite contact size of the indenter tip. The experimental setup consists of a load frame, a freestanding circular thin film membrane, high precision translation stages, and two microscopes. Load frames and freestanding circular thin film membranes were fabricated using standard microfabrication techniques. The load frames consist of fixed-fixed beams with lengths varying from 500 to 3000 microns and widths of 2 to 4 microns. Freestanding circular thin films were fabricated with thicknesses as small as $\sim$90 nm and diameters as high as $\sim$850 microns. High-resolution stages are necessary to align precisely the free standing circular membrane and the load frame. Manual manipulation stages are used for alignment, while a piezo-actuator with a resolution of 0.9nm is used for indentation. Two microscopes are used to simultaneously measure the displacement of the membrane and the load frame. An interferometric microscope is used to image the underside of the membrane and captures the full-field deflection of the freestanding circular thin film membrane during testing. A vernier co-fabricated with the load frame is simultaneously observed by an optical microscope to provide the deflection of the center-point of the fixed-fixed beam. The deflection of the fixed-fixed beam is then converted to a force using non-linear beam theory to a resolution of $\sim$25 nN of applied force. Preliminary experiments were conducted using free-standing gold membranes, where the load-displacement data were captured and compared with a recently developed model. Membranes were loaded beyond their elastic limits to measure the yield strength as a function of membrane thickness. When loaded beyond the elastic limit, these membranes developed complex

buckling fields that validate theoretical predictions.

11:45 AM AA8.13
In-situ SEM and TEM Mechanical Testing of Nanostructures. Yong Zhu and Horacio D. Espinosa; Northwestern University, Evanston, Illinois.

While in-situ measurement of mechanical properties of nanostructures (e.g. nanotubes, nanowires, and ultra thin films) is challenging, significant research efforts are being conducted in this area. The major limitation of the current experimental techniques is that both deformation and force are deduced from the microscopic imaging of specimen and testing structure. This scheme results in the impossibility of continuous observation of the specimen deformation and failure while independently measuring the applied load. In order to overcome this limitation, another approach to measure electronically the applied force has been developed by our group. The novel microelectromechanical system (MEMS) testing stage consists of actuator, specimen and force sensor. Two types of actuators, thermal actuator and comb drive actuator, are used to achieve displacement-controlled and force-controlled actuation respectively. Differential capacitive sensing is used for the force measurement. The thermal actuator has a motion range from tens of nanometers up to 1 micrometer while the comb drive actuator can move up to 4 micrometers. The capacitance change of the force sensor was measured using an integrated circuit (IC) chip, with a resolution of 0.05 femtoFarads. A calibration curve of the capacitance change and sensor displacement for the force sensor was obtained. The stiffness of the force sensor was identified by resonance of the sensor structure completing the calibration process. The force sensor possesses nano-Newton resolution. The accuracy of the testing stage has been demonstrated by testing nanoscale freestanding polysilicon films. Size of the MEMS devices is so small that they can be easily put inside scanning and transmission electron microscopes (SEM and TEM). Experimental setups for both in-situ SEM and TEM testing have been developed. Metallic nanowires were synthesized using anodized aluminum oxide as template. They have been successfully mounted on the testing stage using a nanomanipulator from Klocke Nano-technik. Considerable lower elastic modulus and much higher yield strength compared to the bulk counterparts have been observed in the in-situ SEM testing. Plasticity size effects of these 1-D structures will be discussed in relation to previous work by our group on plasticity size effects in submicron freestanding thin films. In addition, multi-walled carbon nanotubes were tested in-situ the TEM. A fracture strength of 15.84 GPa and a failure strain of 1.56% was measured. These results are in agreement with those previously reported in the literature. However, a new phenomenon was observed during the in-situ experiment. After failure, the graphite shells disappeared. Instead, a large number of nanoparticles (with diameters ranging from 5 nm to 50 nm) embedded in an amorphous matrix were observed. Detailed characterization of this phenomenon is underway and will be reported shortly.

SESSION AA9: Tribology
Chair: A. Ngan
Thursday Afternoon, December 1, 2005
Republic B (Sheraton)

1:30 PM *AA9.1
Dry Friction at the Nano- and Micro-Scale. Kyung-Suk Kim, Division of Engineering, Brown University, Providence, Rhode Island.

Dry friction between an atomically smooth surface of pyrolytic graphite or mica, and a surface of a glass bead coated with various metals is measured with a lateral atomic force microscope. A new method of direct friction-force calibration has been developed to measure the dry friction behavior at the nano- and micro-scale. A diamagnetically levitated graphite sheet is used for the calibration in the lateral force atomic force microscope experiment. The absolutely quatitative measurement shows that the single asperity friction stress increases as the radius of contact increases. The scale-dependent friction stress is then compared with the prediction based on a dislocation-emission model. The comparison shows that the friction stress is sensitive to the environment; the friction in the air is much smaller than that in a vacuum. However, if the normal load is beyond a threshold bvalue, the tribo-chemical wear dramatically increases the friction. In addition to the single-asperity-contact friction studies, the transition behavior of friction from single- to multiple-asperity contacts has been investigated with a glass bead coated with various metals, sliding on an array of multi-wall carbon nano tubes. The experiment shows the transition from the single-asperity adhesive friction to the Amontons-Coulomb type friction. When the normal force increases beyond a threshold value for dislocation movements in the metal coating, the friction coefficient of the multiple-asperity friction increases substantially.

2:00 PM *AA9.2
Wear and Friction Behavior of NiTi Shape Memory Alloys – Phase Transition versus Plasticity. Qingping Sun, Mechanical Engineering, Hong Kong Univ. of Sci. and Tech., Hong Kong, China.

NiTi polycrystalline shape memory alloy has been an excellent candidate material for MEMS in the form of thin film and has been increasingly used as biomaterial such as human implants. In these applications, the wear and friction behavior of the material and devices are very important in enabling new technologies and have become the focus of current research. This talk reports recent experimental study of the wear and friction properties of thin film and bulk NiTi on sub-microscale. Through quantifying the role of phase transformation and its interplay with plastic strain accumulation in the wear and friction processes of the material by nanoindentation and scratch, systematic experimental data and a fundamental understanding for the wear mechanism of the thin film are obtained.

2:30 PM AA9.3
Plastic Deformation in Frictional Sliding Contact of Nanocrystalline Materials. Simon Bellemare, Ming Dao and Subra Suresh; Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Earlier studies have shown that a simple frictional sliding or scratch experiment generates plastic strains of larger magnitude than those obtained in normal indentation. However, there is currently no mechanical model to relate this response to the plastic flow properties of materials. In this work, progress has been made in establishing these relationships and the experimental and computational framework enabled to study the effect of microstructural variables on the plastic deformation behavior of nanocrystalline materials. Finite element methods were used to parametrically study the individual contributions of initial yield strength and plastic strain hardening on the normal force, steady-state friction coefficient and pile-up height. The model was three dimensional to account for the directionality of the plastic flow and adhesive friction with the rigid indenter was incorporated using Coulomb's law. The results were analyzed using dimensionless variables. It is predicted that materials with the same indentation hardness can have a significantly different response in frictional sliding. The computational results are compared with experiments using model material systems with well-known plastic deformation behavior. In an aluminum alloy system, the strain hardening behavior is varied through heat treatments leading to similar indentation hardness. The findings are used to interpret results from simple and repeated frictional sliding experiments on pure and alloyed nanocrystalline nickel with different grain sizes. The effect of alloying on grain growth during repeated frictional sliding experiments is especially addressed.

2:45 PM AA9.4
Nanoscale Wear Testing of Single and Polycrystalline Nickel. Neville Moody[1], Megan Cordill[2], John Jungk[3], Marian Kennedy[4], Soumari Prasad[3], David Bahr[4] and William Gerberich[2]; [1]Sandia National Laboratories, Livermore, California; [2]University of Minnesota, Minneapolis, Minnesota; [3]Sandia National Laboratories, Albuquerque, New Mexico; [4]Washington State University, Pullman, Washington.

Strength, friction, and wear are dominant factors in the performance and reliability of materials and devices fabricated using nickel based LIGA technologies. However, there are few studies addressing fundamental effects of friction and wear on properties and performance of these polycrystalline materials. We have therefore begun a program employing nanoscratch and nanoindentation techniques to define these effects using single crystal nickel and polycrystalline LIGA nickel samples. The use of single crystal samples allows us to define processes controlling polycrystalline behavior. Nanoscratch techniques were used to generate wear patterns as a function of load and number of passes followed by tests on each pattern to determine corresponding coefficients of friction. Nanoindentation was then used to measure properties in each wear pattern. The results showed a much greater degree of wear occurred on the single crystal nickel sample than on the polycrystalline LIGA nickel reflecting the lower hardness of the single crystal nickel. However, the coefficients of friction superimposed, exhibiting the same systematic increase with load and number of scratch passes for each sample. In this presentation, we will use measured hardness values and Johnson's cavity model for plasticity to show that flow stress and the extent of plasticity systematically increase with applied load and sliding cyclic contact for both samples. We will further show that the similarity in the evolution of plasticity leads to a similarity in frictional response between the single and polycrystalline samples.
The authors gratefully acknowledge the support of Sandia National Laboratories. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company for the United States Department of Energy's National Nuclear Security Administration

under contract DE-AC04-94AL85000.

3:30 PM *AA9.5
Atomic Modeling of Adhesion, Adhesive Transfer and Friction at Al/Carbon Interfaces. Yue Qi, Materials & Processes Lab, GM R&D Center, Warren, Michigan.

The unique tribo-chemical properties of crystalline diamond and amorphous diamond-like carbon (DLC) have stimulated substantial interest in their use in a diverse group of applications ranging from NEMS/MEMS devices to tool coatings. In addition to their low friction and high wear resistance, the anti-sticking property of carbon-based materials to the extremely chemical affinitive aluminum has made them desirable coatings for the machining of aluminum. In the present work, various Al/carbon interfaces have been studied using Density Functional Theory (DFT) to reveal the nature of interfacial bonding and strength. Adhesive transfer is explored by subjecting the Al/carbon interfaces to a series of tensile strain increments up to fracture. It has been found that Al tends to transfer to a clean diamond surface, but does not transfer to chemically passivated interfaces; on the other hand, graphite will transfer to Al surface. The effect from the testing atmosphere on the friction behavior of DLC against Al can also be explained through different absorption behaviors of gas molecules at the diamond surface modeled with DFT. These results collectively agree with experimental observations and provide deeper insight and guidance for coating design in situations where adhesion to aluminum is to be minimized or eliminated.

4:00 PM AA9.6
Nanoindentation of Single Crystals: Effects of Interface Friction and Adhesion Energy. Virginie Dupont and Frederic Sansoz; Dept. of Mechanical Engineering, University of Vermont, Burlington, Vermont.

Nanoindentation and scanning probe microscopy are powerful tools to investigate the nanomechanical behavior of structural surfaces, thin films and nanowires. At the nano-level length scale, however, the elastic limit and defects nucleation in those materials are strongly influenced by several factors: tip geometry, tip size, interface friction, and adhesion. Hertzian elastic theory is often used to extract mechanical properties from indentation data, despite common knowledge that this model does not account for interface friction and adhesion. The present paper intends to provide further insight into the elastic deformation and defect nucleation of FCC single crystals via simulations of mechanical contacts with friction and adhesion. Molecular statics and dynamics are used to simulate the indentation of <111> and <112> single crystal surfaces with a 10nm-radius single crystal cylinder. Interface friction and adhesion energy are altered by changing both crystal orientation and interatomic potentials. The simulations are conducted using the EAM potentials for Au, Al, and Cu. The atomistic results are compared to the continuum elastic theories of M'Ewen and Johnson, Kendall and Roberts (JKR) which includes friction and adhesion, respectively. Our atomistic results are in good agreement with the continuum theory at the early stage of deformation, but deviate from this theory near the elastic limit.

4:15 PM AA9.7
Dislocation Dynamics Simulations of Rough Surface Contact. Lucia Nicola[1], Alan Needleman[1], Allan F. Bower[1] and Erik Van der Giessen[2]; [1]Engineering, Brown University, Providence, Rhode Island; [2]Applied Physics, University of Groningen, Groningen, Netherlands.

Due to unavoidable roughness, contact between surfaces is characterized by localized plastic deformation, even under light loading. When the loading is removed this leads to the development of a residual stress state that can promote crack nucleation. Therefore the study of plasticity in rough surface contact is of major importance for understanding friction and wear, as well as contact and fretting fatigue. We carry out simulations of indentation of an infinitely long two dimensional deformable single crystal by a rigid flat indenter. The profile of the crystal surface is taken to be a sinusoidal wave. Plasticity in the crystal occurs by the the collective motion of discrete dislocations. The dislocations are modeled as line singularities in an otherwise isotropic linear elastic medium. A set of constitutive rules is supplied for the glide of dislocations as well as their generation, annihilation and pinning at point obstacles. The solution for the state of stress and deformation is at every increment given as a superposition of two contributions: the known, analytical solution for individual dislocations in infinite space and a non-singular linear elastic, finite element solution that enforces the proper boundary conditions. The sum of these fields incorporates the long-range interactions. The simulations track the evolution of the dislocation structure during loading and unloading.

4:30 PM AA9.8
Tribology of Diamond-Like Nanocomposite Coatings for Ni-Based MEMS: Contact Stress-Materials Damage Relationship Under Sliding Contacts. John Jungk, Joseph R. Michael and Somuri V. Prasad; Sandia National Laboratories, Albuquerque, New Mexico.

Electroformed Ni and Ni alloys are the materials of choice for microelectromechanical systems (MEMS) fabricated by LIGA [(German acronym for) Lithographie Galvanoformug (electroforming)Abformung (molding)]. Although Ni alloys meet many of the structural requirements for MEMS applications, their tribological behavior is of concern for reliable operation. Surface coatings such as diamond-like nanocomposites (DLN) are known to reduce the friction coefficient of bare nickel from 1.2 to less than 0.2. Significant reductions in wear and debris generation were also reported; however, the reliability of the interface between the hard DLN coating and the ductile metal surface is not well understood. In the current study, a series of instrumented indentation tests were performed with a silicon nitride ball at loads ranging from 100 mN to 1 N on both uncoated and 500 nm thick DLN-coated nickel surfaces to determine the maximum contact stress that the DLN coating on Ni surface could withstand. These results are compared with unidirectional linear friction tests using similar silicon nitride balls to understand friction transitions with increased contact stresses. Cross-sections of wear scars were prepared by focused ion beam microscopy and analyzed by electron backscattered diffraction (EBSD) to understand the friction-induced materials damage. The analyses and experimental findings identified three distinct regimes. In low contact stress regimes, deformation in the DLN coating was predominantly elastic, and the coating prevented plastic deformation in the Ni substrate. At intermediate contact stresses, the Ni substrate was plastically deformed resulting in bending of columnar grains, although there was no decohesion of the coating-substrate interface. When the load exceeded a critical value, the higher contact stresses resulted in coating fracture. The implications of these studies on LIGA Microsystems reliability will be discussed. *Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

SESSION AA10: Poster Session: Thin Films and Electronic Materials
Chair: A. Ngan
Thursday Evening, December 1, 2005
8:00 PM
Exhibition Hall D (Hynes)

AA10.1
A Study of Tensile Stress Generation Due to Island Coalescence in Thin Metal Films. Abhinav Bhandari[1], Sean J. Hearne[2] and Brian W. Sheldon[1]; [1]Division of Engineering, Brown University, Providence, Rhode Island; [2]Sandia National Laboratories, Albuquerque, New Mexico.

Stress evolution in thin films has been an extensively studied field for the last few decades. A suggested mechanism for tensile stress generations in Volmer-Weber films is grain boundary formation during island coalescence. In the past, researchers have not been able to measure this stress precisely because the stochastic nucleation of islands results in coalescence over a range of different times and length scales. Hearne *etal.*[1] have demonstrated a technique to control island geometry using selective growth of films on patterned substrates via electrodeposition. Using the same procedure we electrodeposited Ni films on patterned Si (001)substrates to study the dependence of the tensile coalescence stress on growth rate and island size. In these studies, the majority of the tensile stress associated with coalescence occurs after the initial contact of the neighboring islands and the stress reaches a steady state as the films planarize. The steady state stress increases with growth rate for a specific island size and decreases with increasing island size for a fixed growth rate. These experimental results were compared to an analytical model for stress creation after the initial contact of neighboring islands. 1. S.J. Hearne, S.C. Seel, J.A. Floro, C.W. Dyck, W. Fan, S.R.J. Brueck, *J.Appl.Phys.97*, 083530 (2005).

AA10.2
Effect of Adhesion Promoters on Anomalous Subcritical Debonding of Polymer/SiN$_x$ Interfaces. Bree M. Sharratt[1], Brian McAdams[2], Karl Loh[2] and Reinhold H. Dauskardt[3]; [1]Aeronautics and Astronautics, Stanford University, Stanford, California; [2]Zymet, Inc., East Hanover, New Jersey; [3]Materials Science and Engineering, Stanford University, Stanford, California.

Interface integrity can play a crucial role in a variety of manufacturing situations where polymeric and inorganic films are employed in complex structures. Even though interfacial debonding associated with thermal, mechanical, and chemical mismatch is of

considerable technological importance, a complete understanding of the mechanisms that govern debonding of these interfaces is lacking. In the present study, we explore subcritical debonding between a diglycidyl ether of bisphenol F model polymer and a SiN_x thin film. This weakly bonded polymer/inorganic interface was found to be highly susceptible to moisture attack and anomalous near-threshold behavior was observed. The slight dependence of debond growth rates on the magnitude and type of applied loading coupled with high sensitivity to the activity of moisture in the environment was attributed to moisture diffusion to the interface followed by debonding of the polymer layer. A new mechanism to describe the anomoluous threshold crack growth behavior is reported. We then study the effect of interface chemistry by systematically varying the polymer/SiN_x interface by modifying the bisphenol F layer through the addition of adhesion promoting molecules. Three silanes (aminopropyltrimethoxysilane, glycidoxypropyltrimethoxysilane, methacryloxypropyltrimethoxysilane), n-propyl zirconate, and n-propyl titanate were blended into the bisphenol F to make 0.2 wt% epoxy blends. Additional studies were conducted by spinning the adhesion promoters onto the substrate and making specimens with the unmodified bisphenol F layer. We describe the effects of the adhesion promoter on the mechanical properties of the polymer film and discuss the effect on both adhesion and subcritical debonding behavior.

AA10.3
Large Elongation of Metal Interconnects on Elastomeric Substrates due to Out-of-plane Deflection. Teng Li[1], Zhigang Suo[1], Stephanie P. Lacour[2] and Sigurd Wagner[2]; [1]Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts; [2]Department of Electrical Engineering, Princeton University, Princeton, New Jersey.

Flexing, rolling, and even stretching integrated circuits is today a major technology thrust. To be deformable, metal interconnects must elongate by a large amount when the underlying elastomeric substrates are stretched, often repeatedly. Two recent designs have demonstrated remarkable capability, allowing metal interconnects be stretched beyond an elongation of 20%, and over hundreds of cycles. In one design, tortuous metal interconnects are encased in an elastomer. In the other design, distributed microcracks exist in the as-deposited metal interconnects, but ligaments still percolate the interconnects to maintain electrical conductance. Here we provide a fundamental understanding of the large stretchability of metal interconnects on elastomeric substrates. Our finite element simulations reveal that, while the as-deposited interconnects are planar, they deflect out of the plane when the elastomeric substrates are stretched. The out-of-plane deflection allows the metal interconnects to deform mostly elastically, and to snap back upon unloading. By contrast, if the substrates are too stiff, the interconnects are constrained to deform within the plane, leading to the rupture of the interconnects at small elongations. Our study provides guidelines for the selection of geometry and materials of stretchable interconnects.

AA10.4
Intrinsic Strain Generation Mechanisms in Alloy Strengthened Ni. Sean J. Hearne, Jerry A. Floro, Mark A. Rodriguez, Ralph T. Tissot, Collen S. Frazer, Stephen Foiles and Luke Brewer; Sandia National Labs., Albuquerque, New Mexico.

The strain evolution during electrodeposition of NiMn from a sulfamate-based bath was investigated as a function of Mn concentration and current density. The NiMn strain evolution consisted of two regions, an initial transitional strain region followed by a steady-state region that was dependent on deposition rate, similar to the previously reported stress evolution in electrodeposited Ni (Hearne, S. J., Floro, J.A. J. Appl. Phys. 97, 014901-1 (2005)). In-situ stress measurements found that the steady-state stress increases linearly with Mn content. Additionally, ex-situ X-ray diffraction methods showed that addition of Mn, and increased current density during deposition, caused an increase in micro-strain. However, there was no corresponding change in the out-of-plane texture. This implies that there are multiple strain mechanisms active during electrodeposition such as coalescence of grain boundaries and/or point-defect generation. The roles and interactions of these different mechanisms will be discussed. This work was supported by the DOE office of Basic Energy Science. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.

AA10.5
A New Device to Characterize the Mechanical Stress by Packaging Processes. Soeren Hirsch and Bertram Schmidt; FEIT-IMOS, Uni Magdeburg, Magdeburg, Germany.

This paper reports on a new method for estimation and minimization of mechanical stress on MEMS sensor and actuator structures due to packaging processes based on flip chip technology. For studying mechanical stress a test chip with silicon membranes was fabricated. A network of piezo-resistive solid state resistors created by diffusion was used to measure the surface tension pattern between adjacent membranes. Finite element method simulation was used to calculate the stress profile and to determine the optimum positions for placing the resistive network. An increased spreading of MEMS technology constantly requires new and customized packaging techniques while cost pressure remains high and is hardly being met by tailored processes . To still satisfy the demanding criteria of quality and reliability negative effects caused by packaging have to be analyzed and characterized as early as possible. Those are reduced subsequently but not entirely removed by calibration. The combination of both finite element method (FEM) simulation and practical measurements allows the definition of guidelines for positioning sensor structures during the design phase and to significantly reduce residual stress after packaging. The simulated stress distribution across the section of a MEMS structure that has been determined by FEM simulation (ANSYS). The maximum stress area would be the optimum location to place resistors for measuring the stress profile caused by process temperature changes. Using a time-controlled wet-chemical anisotropic tray etching process membranes were created with individual thickness. This allowed the analysis of various stress scenarios. It has been challenging to produce all membranes within one process step. The silicon test chip was contacted using flip chip technology. First measurement results show a good agreement with the simulations. In addition it was possible to define design guidelines for the packaging process and to verify existing concepts. Linking FEM simulation with the measurements of piezo-resistive resistors allowed validation of the used methods as well as of applied load rations and constraints.

AA10.6
Mechanical Behavior of SiO_2-Filled Epoxy Resins at Different Length Scales. Marvin I. Francis and Junghyun Cho; Mechanical Engineering, State University of New York, Binghamton, New York.

The flip-chip packaging system has seen increased use in the electronics industry in recent years. A flip-chip package consists of a silicon die connected to an organic substrate through a solder joint. In order to alleviate thermomechanical stresses induced upon the solder joints during the device operation, an epoxy resin (called 'underfill') is dispensed between the die and substrate. The epoxy often contains silica (SiO_2) beads which help decrease the coefficient of thermal expansion (CTE) of the underfill so that it matches more closely that of the silicon die and substrate. A mechanistic understanding of this SiO_2-filled epoxy underfill is essential to enhance the reliability of overall packaging system. Thus, we employ nanoindentation to analyze mechanical behavior of the underfill materials at nano- and microscales. Specifically, time-dependent deformation such as viscoelasticity, creep, and stress relaxation is systematically examined at various curing conditions through the dynamic nanoindentation by superimposing a small, sinusoidally varying signal on top of a DC signal that drives the indenter motion. One emphasis is given to highlight the effect of the filler size and distribution on localized mechanical behavior of the epoxy resin. In parallel with experimental approaches, indentation simulation using a finite element analysis (FEA) will also be implemented. Further, viscoelastic models developed to interpret the nanoindentation data will be correlated to the corresponding macroscopic behavior of the underfill materials measured from a universal mechanical tester. A connection between different length scales will further enhance our understanding on mechanical performance of the SiO_2-filled epoxy resin.

AA10.7
A Mechanistic Understanding of Bilayer Polymer Coatings Using Nanoindentation. Hyungsuk Lee and Junghyun Cho; Mechanical Engineering, State University of New York, Binghamton, New York.

Polymers occupy a significant fraction of electronic/MEMS packaging materials and their share is expected to grow further. A mechanistic understanding of the phenomena that occurs during deformation of polymer is, however, lacking partly due to their strong time and temperature dependent characteristics. Polymers such as parylene family and polydimethylsiloxane (PDMS) have shown a great potential as surface coatings and thin films. Given that, we exploit a two-ply ('bilayer') coating structure consisting of these two polymers (parylene on PDMS) in order to maximize mechanical performance as a protective coating. For this purpose, $in-situ$, dynamic nanoindentation is employed to study the aforementioned temporal mechanical response of polymers at various temperatures. The main goal is to develop the underlying nano- and micromechanics models to highlight mechanical performances of the bilayer polymer coating. These mechanical behaviors will be correlated with the surface structure and properties of the PDMS pre-layer, wherein the parylene-PDMS adhesion and viscoelasticity will be examined through nanoindentation measurements. A better mechanistic understanding

of the interface properties, as well as the substrate effect is essential to achieve desirable macroscopic properties that would in turn offer *innovative* solutions to the challenges found in the current packaging technologies.

AA10.8
A Study on the Mechanisms of Generation and Growth of Stress Induced Voiding in Cu Interconnect. Hyo-Jong Lee[1,2], Heung Nam Han[1], Suk Hoon Kang[1], Kyu Hwan Oh[1], Sun-Jung Lee[2] and Hong-Jae Shin[2]; [1]Material Science and Engineering, Seoul National University, Seoul, Seoul, South Korea; [2]Advanced Process Development Team, System LSI Business, Samsung Electronics Co., Ltd., Youngin-city, Kyunggi-do, South Korea.

Since IBM published the copper integration in 1997, almost all chipmakers have adopted the copper damascene process in their logic devices of 130nm design rule. Moreover, beyond 90nm generation, low-k materials will also be adopted with the copper interconnect. These replacements in conducting material and dielectric material need various test items for reliability, such as EM(electromigration), BTS(bias temperature stressing) and TDDB(temperature dependent dielectric breakdown). In addition to these three test items, HTS(high temperature storage) test becomes very important because void and hillock are generated by heat budget and cause interconnection failure. HTS test in the copper interconnect is to estimate mainly void generation and its growth after heat treatment, and it is reported that such voids happen in the area where via contacts wide metal line, and many simulation data for thermal stress show stress concentration near the via. This result seems to be a similar phenomenon as the SIV(stress induced voiding) in aluminum interconnect. Recently, Lee reported that the voids in wide pattern were randomly generated and many of them were already generated before via etch process. Such voids seemed to be generated during ESL(etch stopping layer) and IMD(intermetallic dielectric) depositions. Therefore, interconnection failure in the chain pattern of wide lines happens because stochastically one of thousands of vias may unfortunately land down on a void in the wide line. This study is to understand the mechanisms of void generation and growth. Crystallography analysis by EBSD(electron backscatter diffraction) shows that a void is generated at triple junction of grain boundaries, not of twin boundaries. Additionally, it is possible to measure the crystalline structure of surface covered with the void. Under the consideration of the grain structures that are rebuilt from EBSD analyses, we calculate the stresses by using a finite element method(ABAQUS). That result agrees well with the measurement result.

AA10.9
Step-bunching on Axisymmetric Crystal Surfaces.
Pak-Wing Fok, Dionisios Margetis and Rodolfo Ruben Rosales; Mathematics, MIT, Cambridge, Massachusetts.

We study step bunching on crystal surfaces from a dynamical standpoint, accounting for diffusion of adatoms across terraces and attachment-detachment of atoms at step edges in the simplest non-trivial setting: that of an axisymmetric crystal with circular steps and a single facet. First, we show by solving numerically equations for the step motion that, for pure attachment-detachment limited (ADL) kinetics, step bunches ALWAYS form, for ANY step-interaction parameter, provided that a sufficiently long time has passed and the initial step spacing is suitably chosen. This property is consistent with a scale invariance of the governing equations. Second, we find a scaling law for the step bunch width with the step-interaction parameter. We explain this scaling analytically on the basis of a continuum equation for the Lagrangian coordinates of step motion. Furthermore, we extend these results to non-conical initial shapes. Last, we study the combined effect of ADL and terrace diffusion limited (TDL) kinetics: We show that, for small values of the step-interaction parameter and surface regions close to the facet edge, the step kinetics is primarily ADL. By contrast, sufficiently away from the facet the step kinetics appear to be primarily TDL. As the step-interaction parameter decreases, step bunching spreads throughout the surface and the entire system of steps is driven towards ADL kinetics.

AA10.10
Modeling of Diffusional Flow and Grain Boundary Sliding in Cu Interconnects. Vasyl Grychanyuk, Todd S. Gross and Igor Tsukrov; Mechanical Engineering, University of New Hampshire, Durham, New Hampshire.

We employ the finite element technique to model diffusion-based deformation and stress relaxation that occurs in Cu-damascene interconnects during thermal cycling. The difference in coefficients of thermal expansion (CTE) between the conductor, liner, and dielectric will generate stresses during thermal processing. We consider the situation where inelastic strain by dislocation motion is inhibited by the small size of the interconnect lines and that the principal mechanisms of transient inelastic deformation are stress-driven diffusional flow of vacancies and diffusion-accomodated interfacial sliding. Following the classical models of Nabarro-Herring and Coble diffusional creep, we consider that vacancy diffusion occurs through the grain bulk as well as along the grain boundary region of enhanced diffusivity with the thickness on the order of several layers of atoms. The formulation is incorporated into the commercially available finite element software package MSC.Marc. We validate the finite element technique by comparison to theoretical predictions for simple geometries and will compare our results to a similar model presented by Garikipati et.al. We also present the isothermal stress relaxation response of simple interconnect geometries subjected to a step temperature change. We find that the inelastic strain is highly localized in the grain boundaries for small structures.

AA10.11
Subsurface Observation and Numerical Modelling of Microstructural and Contact Geometry Effects on Indentation Failure Mechanisms in Columnar-Grained TiN Coatings.
Mark Hoffman[1], Matthew Tilbrook[1], Sanjit Bhowmick[2], Zonghan Xie[1], Vikram Jayaram[2] and Sanjay Biswas[2]; [1]School of Materials Sci. & Eng., The University of New South Wales, UNSW, New South Wales, Australia; [2]Indian Institute of Science, Bangalore, India.

Titanium nitride coatings are commonly used for improving the wear resistance of abrasive surfaces but conjecture exists as to the optimum coating thickness and microstructure for best performance. TiN films produced by physical vapour deposition (PVD) tend to exhibit a columnar grain structure, with attendant anisotropies in elastic and fracture properties, but computational simulations to date have treated TiN films as homogeneous and isotropic. Mechanical behaviour of TiN is usually characterised using nanoindentation, as is typical with most thin film systems. In this work numerical modelling, incorporating the coating microstructure is used to explain the various observed subsruface fracture processes of the coating under spherical indentation. Subsurface observations using focussed ion-beam milling beneath indentations reveal that relatively benign intercolumnar sliding between grains exists in some regimes while in other situations gross cracking may occur. Numerical simulations of deformation/damage mechanisms during the nanoindentation of TiN coatings on ductile substrates have been developed which explain this behaviour. Intergranular sliding was incorporated into the model through the use of anisotropic property definitions and nodal coupling. Substrate and coating properties were calibrated by comparison with experimental nanoindentation results. Effects of coating thickness, contact radius, substrate ductility, intergranular strength and residual stresses upon fracture and deformation were established. It is revealed that the performance of a coating is governed by envelopes of these parameters.

AA10.12
Continuum Theory of Evolving Crystal Surfaces: Boundary Conditions at Circular Facets. Dionisios Margetis and Pak-Wing Fok; Mathematics, MIT, Cambridge, Massachusetts.

The evolution of facets on crystal surfaces is studied as a free-boundary problem from a continuum viewpoint via formulating and testing effective boundary conditions at facet edges. To elucidate the role of such conditions analytically we focus on the simplest, non-trivial setting: the morphological relaxation of axisymmetric crystals with a single facet, in the presence of diffusion of adatoms across terraces and attachment-detachment of atoms at steps. First, a boundary-value problem is formulated for a highly nonlinear partial differential equation (PDE) satisfied by the slope profile outside the facet: We consider two different sets of boundary conditions, one stemming from equilibrium thermodynamics and another accounting for the motion of the first few steps. Second, PDE solutions under each of these condition sets are compared with results of simulations following the motion of atomic steps for various initial profiles and long times so that shapes become self-similar. It is shown that a continuum approach in such parameter regimes can yield reliable predictions when supplemented with boundary conditions of the second set: current continuity and the condition that the facet height drops by integral multiples of the step height, previously mentioned, but not implemented, by Israeli and Kandel [Phys. Rev. B 60, 5946 (1999)]. The role of thermodynamics in these conditions is discussed.

AA10.13
Modified Kinetic Model for Step-Edge Dynamics: Modeling, and Derivation of Step Line Tension. Russel Caflisch[1] and Dionisios Margetis[2]; [1]Mathematics, UCLA, Los Angeles, California; [2]Mathematics, MIT, Cambridge, Massachusetts.

This talk describes a kinetic model for the dynamics of a step edge, which modifies a previous model [Caflisch et al., Phys. Rev. E 59, 6879 (1999)] to render it exactly conservative. The formulation includes attachment and detachment of atoms at step edges, diffusion along the edge, attachment at kinks, and creation and coalescence of

kinks. For consistency with thermodynamics, an energy and an entropy are defined in terms of the terrace-adatom, edge-adatom and kink densities, and the resulting free energy for this model is shown to be monotonically decreasing with time. The Gibbs-Thomson formula and the corresponding line tension of a step as a function of the step orientation are derived from the model analytically using perturbation theory. These results are compared with different, phenomenological approaches.

SESSION AA11: Coatings and Multilayers
Chair: Y. T. Cheng
Friday Morning, December 2, 2005
Republic B (Sheraton)

8:30 AM AA11.1
Mechanical Properties of Nanometric W/Cu Multilayers.
Baptiste Girault[1], Damien Faurie[1], Pascale Villain[1], Pierre-Olivier Renault[1], Eric Le Bourhis[1], Philippe Goudeau[1], Frederic Badawi[1] and Veronique Pelosin[2]; [1]Laboratoire de Metallurgie Physique UMR 6630 CNRS, Universite Poitiers, Futuroscope-Chasseneuil Cedex, France; [2]Laboratoire de Mecanique et Physique des Materiaux UMR 6617 CNRS, ENSMA, Futuroscope-Chasseneuil, France.

Surfaces contribution becomes preponderant in nano-sized crystals yielding deviations from the average mechanical behavior of the material [1]. Multilayer structures offer the opportunity for studying the mechanical properties of low dimension systems. In order to analyze the elastic behavior of nanostructured W layers, W/Cu multilayers with period thicknesses ranging from 24 down to 1.7 nm and different W/Cu thickness ratios have been prepared by ion beam sputtering and characterized using x-ray reflectometry, x-ray diffraction, instrumented indentation and energy dispersive analysis in a Scanning electron microscope. The elastic behaviors of W sub layers (and also Cu for the highest period) have been analyzed using a new method combining X-ray diffraction and tensile testing that is phase sensitive [2]. Elastic response is observed to be well below that expected from a simple rule of mixture. In addition, recent EXAFS measurements [1] indicated that surface alloying may occur in tungsten sub layers for the lowest periods and for equiatomic composition. A possible correlation between these two features is discussed in view of complementary experiments made after post annealing of the specimens. The behavior was observed to depend on the period and the W/Cu thickness ratio of these multilayers as well. The overall obtained results are commented in view of the previously published ones. [1] Goudeau P., Villain P., Renault P.-O., Badawi K.-F., Girardeau T., Elastic constants investigation by x-ray diffraction of in situ deformed metallic multi layers, Scripta Materiala 50 (6) (2004) 723-727. [2] Badawi K.F., Villain P., Goudeau P., Renault P.-O., Measuring thin film and multilayer elastic constants by coupling in situ tensile testing with x-ray diffraction, Applied Physics Letters 80 (25) (2002) 4705-4707.

8:45 AM AA11.2
Analytic treatment of metallic multilayer strength at all length scales.
Lei Fang and Lawrence H. Friedman; Engineering Science and Mechanics, Penn State University, University Park, Pennsylvania.

Metallic multilayers can be used as ultra-high strength coatings. They exhibit a very pronounced size-effect where the mechanical strength depends on the layer thickness. Traditionally, the Hall-Petch relation is used to describe the size effect. The Hall-Petch Relation is based on dislocation pileup theory, which states that the macroscopically observable strength is determined, by dislocation obstacles and stress multiplication from pileups. However, more rigorous application of dislocation pileup theory as applied to multilayers predicts significant deviation from the Hall-Petch relation due to elastic inhomogeneity, discreteness of dislocations and dislocation source operation. The necessary modifications to the Hall-Petch Relation are presented. An analytic formula accounting for these effects can only be obtained in a piecewise fashion. The variation of strength with layer thickness must be broken down into four length-scale regimes, and a simple analytic formula is obtained for each regime. This formulation allows one to bridge the length scales and predict multilayer strength from a microscopic parameters (interface strength and dislocation source characteristics) and fundamental material parameters (elastic moduli and crystal structure).

9:00 AM AA11.3
On Dislocation Mechanisms in Metallic Nanoscale Multilayers: Modeling and Discrete Dislocation Simulations.
Firas Akasheh[1], Hussein M. Zbib[1], Richard G. Hoagland[2], Amit Misra[2] and John P. Hirth[2]; [1]Mechanical and Materials Engineering, Washington State University, Pullman, Washington; [2]Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, New Mexico.

The unusual high strength of metallic nanoscale multiayers, approaching the theoretical strength of the component metals, is drawing increasing interest motivated by its scientific and technological implications. Extensive experimental and theoretical studies have shown that as the individual layer thickness is decreased to the range of tens of nanometer the strengthening effect can not be explained by the classical Hall-Petch relation, indicating that different strengthening mechanism(s) come into play. Furthermore, studies have shown that this strengthening trend becomes weaker and in fact may reach a maximum when the layer thickness is in the few nanometers range. Strong evidence indicates that individual dislocation-dislocation and dislocation-interface interactions become the most significant factor dictating the strength in this range of layer thicknesses. In this work, full three-dimensional discrete dislocation dynamics simulations are conducted to investigate several dislocation interaction mechanisms observed experimentally in Ni-Cu multilayers and theoretical models for the strength of multilayers based on such mechanisms are developed and verified. This includes the effects of coherency stresses, misfit dislocation content, and interface properties on the critical stress for threading dislocation motion and activation of dislocations sources as a function of the layer thickness. Also investigated is the conditions under which slip is transmitted from one layer to the next across the interface.

9:15 AM AA11.4
Multiscale Simulation of Interface Crack Growth in The Metal/Ceramic Multilayers.
Yueguang Wei, Institute of Mechanics, Chinese Academy of Sciences, Beijing, Beijing, China.

Crack growth along a metal/ceramic interface within a multilayer material is analyzed under different length scales. A remarkable characteristic of the crack growth in the multilayer material is that the crack tip constraint effect is important. The crack-tip constraint effects (or T-stress effects) on the elastic-plastic fracture behavior in conventional material and in strain gradient material are analyzed in the present study. The T-stress effects on the stress distributions along the plane ahead of the stationary and growing interfacial crack tip are analyzed. For the steadily growing crack, the T-stress effects on the steady-state fracture toughness are analyzed by adopting both the embedded fracture process zone model and the dislocation-free zone model. In addition, the analysis for the growing crack is applied to an interfacial cracking experiment for a ceramic/metal/ceramic three-layer system, and through comparing the simulation result with experimental result the material length-scale parameter appeared in the strain gradient plasticity theory is predicted.

9:30 AM AA11.5
Molecular Dynamics Simulation of Nano-indentation of Carbon Coated Monocrystalline Silicon.
Davy Wun Chet Cheong and Liangchi Zhang; Mechanical Engineering, University of Sydney, Sydney, New South Wales, Australia.

This paper presents the molecular dynamics (MD) simulation of nano-indentation of diamond-like carbon (DLC) coating on silicon substrates. It is found that the mechanisms of nano-indentation of coated systems on the nanometre scale defers considerably from the same process on the micrometre scale. The coating thickness affects the mechanisms of plastic deformation both in the coating and the substrate. The different modes of plastic deformation are described in this paper. The macroscopic behaviour coatings have been well documented and studied using continuum mechanics. However deformation mechanisms have been shown to be very different on the nanometre scale. A full understanding of the mechanical behaviour of diamond coating on the nanometre scale is an essential issue in such application In this present study, four distinct failure mechanism of coating and substrate due to nano-indentation is observed :- (i) When the ratio of thickness of coating to indenter radius (= t/R) is = 0.35. It is found that the deformation of substrate is almost identical to that in silicon due to indentation without the carbon coating. (ii) When t/R=0.7, it is found that the substrate requires higher indentation load to yield compared to the case without coating due to the thicker coating. The substrate experience plastic deformation before there is any plastic deformation in the coating. (iii) When t/R=1.4, it is found that the coating experience plastic deformation before the substrate. The substrate also experience plastic deformation when the indenter is further loaded. (iv) When t/R=2.8, it is found that there is no plastic deformation in silicon substrate. The mechanism of plastic deformation for the carbon coating is similar to the plastic deformation of carbon specimen due to nano-indentation. Noting the force at which the coating and substrate experiences plastic deformation, a failure map can be plotted. Hence the plastic deformation of a diamond coated silicon system can be defined using the failure map provided the scale of analysis is small enough to ensure that crack formation and dislocations are not initiated.

9:45 AM AA11.6
Nanoindentation-Induced Damage and Modelling of Diamond-Like Carbon Coating on Ductile Substrates.
Rajnish Kumar Singh[1], M. T. Tilbrook[1], Z. H. Xie[1], A. Bendavid[2], S. Yew[1], P. Martin[2], P. Munroe[1] and M. Hoffman[1]; [1]Material Sci. & Engg., UNSW, Sydney, New South Wales, Australia; [2]Division of Industrial Physics, CSIRO, Sydney, New South Wales, Australia.

A diamond-like carbon (DLC) thin film was deposited onto a stainless steel substrate using plasma enhanced chemical vapour deposition (PACVD) method. Nanoindentation was used, with the support of focused ion beam (FIB) technique, to investigate contact-induced deformation and fracture in this coating system. Following initial elastic contact between the coating and indenter and the plastic yield of the substrate, pop-ins were observed in the load-displacement curve, indicative of coating fracture. FIB cross-sectional images of indentations revealed the presence of, ring, radial and lateral cracks at and above the critical load of first pop-ins and radial and ring cracks even at much lower load than the critical load. The three dimensional nature of these cracks was imaged through the use of tomographic techniques. Finite element modelling was employed to calibrate the properties of the substrate and the film, by fitting the predicted load-displacement curves to experimental data. Then, based upon the experimental observations of damage evolution in this coating system, the stress distributions that may be responsible for initiation of ring, radial and lateral cracks in the coating were calculated. Furthermore, the effects of substrate yield strength and coating residual stresses on the formation of these cracks were investigated and implications for future coating design considered.

10:30 AM AA11.7
Inelastic Deformation Mechanisms in Thermal Spray Metallic Coatings. W. Brian Choi[1], Lubos Prchlik[2], Andrew Gouldstone[1] and Sanjay Sampath[1]; [1]Materials Science and Engineering, Stony Brook University, Stony Brook, New York; [2]Skoda, Plzen, Czech Republic.

Thermal sprayed (TS) metallic coatings are widely used in a number of applications including tribological protection and bondcoats for thermal barrier coatings (TBCs). For the former, performance against wear, erosion and foreign object damage is directly related to high-strain inelastic behavior. For the latter, flow behavior is directly related to propensity for rumpling and thus TBC spallation, and is thus of critical importance. In addition, an emerging application for TS metals is mesoscale electronics in harsh environments (e.g., embedded strain gages, antennas). For this, understanding of inelastic deformation during cyclic loading and its effect on functional behavior is crucial. To date, understanding of yield and post-yield phenomena in TS materials is limited to e.g., hardness measurements and loads to failure. In this talk, we will present results from experimental and modeling efforts to elucidate the mechanisms of inelasticity in TS metallic coatings. First, we describe a simple method, based on empirical work by Tabor, for converting Brinell hardness measurements to stress-strain curves. Using this method, results of indentation can thus be used to quantify mechanical behavior of coatings deposited by different processes, and subjected to post-processing treatments, providing a powerful supplement to microstructural characterization. Second, we show how observation of surface and sub-surface deformation (using profilometry and strain mapping) is used to differentiate the contributions from splat distortion and splat-splat sliding, to inelastic deformation under indentation. Finally, we discuss results from in-situ substrate curvature methods designed to extract the in-plane behavior of TS coatings, providing insight into anisotropy and size-effects in these materials. Acknowledgement: Supported through NSF MRSEC award DMR 0080021.

10:45 AM AA11.8
Contact Deformation of Tin Coatings on Metallic Substrates. Vikram Jayaram[1], Sanjith Bhowmick[1], Souvik Math[2] and Sanjay Kumar Biswas[2]; [1]Department of Metallurgy, Indian Institute of Science, Bangalore, Karnataka, India; [2]Mechanical Engineering Department, Indian Institute of Science, Bangalore, Karnataka, India.

Recent developments in the contact deformation and fracture of columnar TiN coatings are reviewed. It is shown that columnar films display two regimes of responses: one dominated by columnar sliding at a critical shear stress which is determined substantially by the residual stress in the film, and the other, more damaging response, characterized by fracture. The transition to cracking modes of response is aided by a soft substrate and a thick film and can be understood from a relative comparison of the driving forces for the different modes by analytically simulating the response of an elastic bi-layer to Hertzian loading. The above comparison suggests that the relative success of columnar films, vis–vis amorphous or equi-axed films, is probably due to the existence of this relatively benign mode of columnar shear. The implications for optimal coating design are also discussed.

11:00 AM AA11.9
Thin films of super-hard cubic Zr_3N_4 stabilized by stress. Husnu Emrah Unalan and Manish Chhowalla; Materials Science and Engineering, Rutgers University, Piscataway, New Jersey.

The deposition and characterization of super-hard cubic Zr_3N_4 thin films is described [1]. The films are deposited using a novel but industrially viable modified filtered cathodic arc (FCA) method which allows unprecedented control over the plasma parameters which is essential for the deposition of the c- Zr_3N_4 phase [2]. The Zr-N thin films deposited using the modified FCA have Zr_3N_4stoichiometry and undergo a phase transformation from orthorhombic to cubic above a critical stress level of 9 GPa as determined by x-ray diffraction and Raman spectroscopy. The c- Zr_3N_4 films are significantly harder ($\sim$ 36 GPa) than both the orthorhombic Zr_3N_4 and ZrN films ($\sim$ 27 GPa). The c- Zr_3N_4thin films are also transparent with an absorption edge at 1.6 eV. Our results indicate that the cubic phase is stabilized by the large stress and high temperature in the growth zone which create suitable thermodynamic conditions for stabilization of the meta-stable phase. The ability to deposit this material directly onto components as a thin film will allow its use in wear and oxidation resistant applications. 1. M. Chhowalla, H.E. Unalan, Nature Materials 4 (2005) 317-322. 2. M. Chhowalla, Applied Physics Letters, 83 (8) (2003) 1542.

11:15 AM AA11.10
The Effect of Ar Pressure on Mechanical Properties of Magnetron Sputtered TiAlCr Coatings. Xiao Li[1], Feng Huang[1], Mark G. Calhoun[2] and Mark L. Weaver[2,1]; [1]Center for Materials for Information Technology, The University of Alabama, Tuscaloosa, Alabama; [2]Department of Metallurgical and Materials Engineering, The University of Alabama, Tuscaloosa, Alabama.

The effect of Ar pressure on residual stress, nanohardness and biaxial modulus of magnetron sputtered TiAlCr coatings was investigated. The stress was measured by the curvature method, and a peak at the Ar pressure of about 12.5 mTorr was observed. The hardness and the modulus, determined through nanoindentation tests, were found to decrease with the increase of Ar pressure. Cross-section microstructural characterization revealed the more distinct columnar structures with the increase of Ar pressure. A discussion is conducted on the correlation of Ar pressure to the kinetic energy of sputtering pieces, the microstructural evolution, the resultant mass density and mechanical properties.

11:30 AM AA11.11
On the volumetric recovery and fleeting hardness of time-dependent materials (polymers). Catherine A. Tweedie and Krystyn J. Van Vliet; Department of Materials Science & Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

As there currently exist few means to quantify the mechanical properties of nanoscale, confined polymeric volumes such as as-deposited thin films and biological substrata, nanomechanical contact approaches such as nanoindentation are applied with increasing frequency. However, time-independent analyses appropriate for metals are still utilized to estimate the plastic strength of polymers via indentation hardness H_i. This metric of strength is the ratio of maximum applied load to contact area of the corresponding plastically (permanently) deformed volume, which is thus assumed to remain constant upon full unloading of the material surface. Here, we assess the validity of this assumption for bulk polymers by measuring the volumetric recovery of nanoindentations as a function of time up to 48 hrs post-indentation via atomic force microscopy. This indentation volume was found to recover substantially and in a manner correlative with bulk mechanical properties and monomer structure for polyethylene (PE), and amorphous polystyrene (PS) and polycarbonate (PC), and three distinct phases of recovery are delineated. The observed changes in depth and volume post-nanoindentation have direct implications regarding the accuracy of H_i as an estimate the mechanical strength of synthetic and biological polymers: To maintain a 10% error tolerance in calculated H_i, the contact depth may not vary more than 33%, indicating that the hardness value would be valid for only 5 min to 3.5 days post-testing for the polymers considered.

11:45 AM AA11.12
Mechanical Properties of Photopolymer Microstructured Films. Taeyi Choi[1], Ji-Hyun Jang[1], Chaitanya K. Ullal[1], Melburne C. Lemieux[2], Vladimir V. Tsukruk[2] and Edwin L. Thomas[1]; [1]Institute for Soldier Nanotechnologies, Materials Science and Engineering, MIT, Cambridge, Massachusetts; [2]Materials Science and Engineering, Iowa State University, Ames, Iowa.

The mechanical behavior of a two-dimensional polymer microlattice with six-fold symmetry fabricated via laser interference lithography

was investigated. Contrary to the uniform distribution of the mechanical properties in traditional MEMS structures, the elastic properties of photopatterned structures in SU8 films exhibit a microscale distribution governed by the symmetry of the initial light intensity distribution controlling the crosslinking reaction. The maximum elastic modulus 1.5 GPa occurs at the lattice nodes corresponding to the local maximum of the light intensity and the lower value of modulus, 1.1 GPa, is reached at the midpoint between neighboring nodes. In addition to the spatial distribution of the elastic modulus of the two-dimensional photopatterned polymer film, the macroscopic quasistatic mechanical properties of the two-dimensional and three-dimensional microtrusses were studied by peeling the film off of its support. A variety of plastic and fracture responses were evident indicating that microstructured films exhibit both size and symmetry related properties.