SYMPOSIUM W

Multiscale Phenomena in Materials–Experiments and Modeling Related to Mechanical Behavior

April 22 – 24, 2003

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as Volume 779
of the Materials Research Society
Symposium Proceedings Series

* Invited paper

SESSION W1: MULTISCALE MODELING OF PLASTIC DEFORMATION I
Chairs: David H. Lassila and Kevin J. Hemker
Tuesday Morning, April 22, 2003
Franciscan II/III (Argent)

8:30 AM *W1.1
MULTISCALE MODELING OF MATERIALS STRENGTH: CURRENT STATUS AND FUTURE DIRECTIONS.
Tomas Diaz de la Rubia, Chemistry and Materials Sciences Directorate, Lawrence Livermore National Laboratory, University of California, Livermore, CA.

One goal of the Computational Materials Science effort at LLNL is to develop experimentally validated models of strength of materials under extreme conditions. Strength of materials is described naturally in terms of complex multiscale behavior crossing over from the quantum mechanics of electrons to the continuum mechanics of macroscopic objects. The effort at LLNL is driven by the requirements of the Advanced Strategic Computing Program within DOE/NNSA, and is a highly collaborative parnership with US academic institutions, including multiple experimental efforts. As such, the effort has accumulated the brain mass necessary for the development of a practical multiscale capability for predictive modeling of material strength, and while progress is tangible, the ultimate goal is still elusive. This talk will report successes and pitfalls on this path and propose a few new directions that we deem worthy of further development. In particular, we will highlight the importance of establishing accurate links between the models of varying degree of detail, such as QM/DFT and MD, MD and DD, DD and continuum. We will also emphasize the critical role of multiscale experiment in making the Program successful.

9:00 AM *W1.2
MODELING OF ENSEMBLE-CONTROLLED PLASTIC DEFORMATION BEHAVIOR IN METALS. Michael Baskes, Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM.

The methods to model plasticity phenomena in metals have traditionally focused on either atomic-scale (e.g., molecular dynamics) or micro-scale (e.g., dislocation dynamics) or macroscopic continuum-scale. This talk will present an overview of recent work in our research group that uses experimental data from mechanical tests and transmission electron microscopy (TEM) characterization of the evolution of ensembles of defects at different length scales to bridge the length scale gaps between these modeling methods. The effects of strain path changes on the mechanical response of fcc metals will be used as an example to illustrate how the relevant quantitative parameters from dislocation substructures, obtained from TEM or micro-scale simulations, can be used as inputs for the continuum models. The links between atomic and micro-scale simulations will also be discussed. Detailed presentations of these results will made by the individual investigators of our research group in this symposium. This research is funded by US Department of Energy, Office of Basic Energy Sciences.

9:30 AM *W1.3
OBSERVATIONS OF DISLOCATION STRUCTURES DEVELOPED DURING DEFORMATION OF MICRO AND NANO-SCALE METALS. Darcy A. Hughes, Materials and Engineering Sciences Center, Sandia National Laboratories, Livermore CA.

Quantitative measurement and analysis of structural parameters have shown for a variety of metals and processes that the microstructural evolution follows a universal path of grain subdivision down to the nanoscale. This behavior has allowed an analysis of the formation and evolution of graded nanoscale structures produced by sliding. Transmission electron microscope (TEM) studies of such structures show the dominating role of dislocations in the development of fine scale deformation microstuctures.

10:30 AM *W1.4
DISLOCATION SELF-PATTERNING AND RECOVERY UNDER SINGLE SLIP: MODELING MICROMECHANISMS FROM EXPERIMENTAL OBSERVATIONS. Patrick Veyssiere and Yu-lung Chiu, LEM, CNRS-ONERA, Chatillon, FRANCE; Fabienne Gregori, LTPCM, University of Paris-Nord, Villetaneuse, FRANCE.

At low temperature, dipolar interaction is the driving force for self-patterning under single slip conditions. The process starts with the spontaneous generation of strings of prismatic loops created by localized cross-slip annihilation. There is no simple diffusion-free mechanism that can engender an isolated prismatic loop, while loop strings should be encountered in any crystal that enables cross-slip. String generation provides a means for dislocation ensembles to bifurcate from homogeneous displacement to gradual congregation into cell walls. Strings allow for dislocation recovery, hence offering an alternative solution to the questionable spontaneous climb process of edge dipoles. Detailed analysis of microstructural organization in crystal deformed monotonously or cyclically in single slip will be provided. There is not much in common between simulations and experimental observations of debris.

11:00 AM *W1.5
DISLOCATION BEHAVIOR DURING DEFORMATION - COMBINING EXPERIMENTS, SIMULATION AND MODELING.
I.M. Robertson and J. Robach, Dept. of Mater. Sc. and Engin., Univ. of Illinois, Urbana, IL; B. Wirth and A. Arsenlis, Lawrence Livermore National laboratory, Livermore, CA.

The changes in mechanical properties of irradiated materials are characterized by a loss of ductility and an increase in the yield strength to the point where a yield drop occurs even in FCC materials. Microstructurally, the deformed material shows the formation of channels from which the radiation defects have been annihilated. Current models are not able to predict the observed macroscopic response. We have combined deformation experiments performed in situ in the transmission electron microscope with molecular dynamics computer simulations to determine the mechanisms by which glissile dislocations interact with and annihilate the defects. This has revealed a wide range of values for the defect pinning strength and has shown that a single interaction is not always sufficient to annihilate a defect. The experiments show that dislocations generated from grain boundaries and other stress concentrators, and not preexisting dislocations, are responsible for creating the channels. Based on these observations a dispersed-barrier hardening, we have developed a crystal plasticity model in which the influence of the radiation defects and dislocation density are combined. The resulting model predicts the observed behavior, including the apparent yield drop at high defect densities.

11:30 AM *W1.6
HARDENING IN MULTISLIP CONDITIONS: THE LOST INTERACTION.
Ronan Madec, DPTA/SPMC, CEA, Bruyeres-le-Chatel, FRANCE; David Rodney, GPM2-INPG, Domaine Universitaire, St. Martin d'Heres, FRANCE; Thierry Hoc, MSSMat, Ecole Centrale Paris, Chatenay Malabry, FRANCE; Benoit Devincre and Ladislas Kubin, LEM, CNRS-ONERA, Chatillon, FRANCE.

This work deals with an interaction between dislocations that seems to have been forgotten when the "forest model" was established fifty years ago. Since then, it is understood that dislocations interactions and intersections govern the flow stress of fcc crystals. This is manifested by a traditional relation between stress and the square root of the dislocation density. Recent studies, involving atomistic as well as mesoscale simulations have confirmed that forest hardening can be investigated within a good approximation within a purely elastic framework. In parallel, the basic scaling law of the forest has been further discussed with the help of parameter-free mesoscale simulations. This work has now been expanded to include a more detailed description of forest hardening. The latter accounts for the interaction of slip systems taken two by two, and is more suited for the continuum modeling of mechanical properties. The measurement of the six interaction coefficients confirms the hierarchy established from latent hardening tests for five of them: two dipolar interactions and three types of junctions. However, the sixth interaction, the so-called colinear interaction, appears to be by far the strongest one: its intrinsic strength is more than six times the one associated with the Lomer or Lomer-Cottrell lock. The colinear interaction, which has been seldom considered in the literature, occurs between dislocations of same Burgers vector gliding in two different slip planes, each being the cross-slip system of the other. A detailed study of this interaction is presented, based on atomistic simulations, elastic calculations, and several types of mesoscopic simulations. The origin of its strength is explained, and consequences regarding microstructural behavior and mechanical properties are discussed.

SESSION W2: MULTISCALE MODELING OF PLASTIC DEFORMATION II
Chairs: Lyle E. Levine and Hussein M. Zbib
Tuesday Afternoon, April 22, 2003
Franciscan II/III (Argent)

1:30 PM *W2.1
DISCRETE DISLOCATION AND NONLOCAL CONTINUUM PLASTICITY MODELING OF INDENTATION.
Erik van der Giessen, Univ of Groningen, Dept of Applied Physics, Groningen, THE NETHERLANDS; Eduardo Bittencourt, Universidade Federal do Rio Grande do Sol, BRAZIL; Alan Needleman, Brown Univ, Div of Engineering, Providence, RI.

Indentation experiments clearly show size effects related to plasticity in small confined volumes and various theories have been used to explain the indentation size effect. Here, we analyze a two-dimensional indentation model using two nonlocal plasticity frameworks, each of which has been shown previously to predict a range of size effects in various boundary value problems. One of these –discrete dislocation plasticity– is inherently nonlocal because it describes plastic deformation through the motion of a large number of discrete dislocations. The other framework is the plastic-strain gradient, continuum crystal plasticity theory proposed by Gurtin (2001). Previous work has shown that Gurtin's theory is capable of representing size effects predicted by discrete dislocation plasticity for a metal-matrix composite and for a constrained single-crystal layer. The issue we address here is the extent to which the discrete dislocation indentation size effect is also captured by Gurtin's theory.

2:00 PM *W2.2
A COUPLED ATOMISTIC AND DISCRETE DISLOCATION PLASTICITY STUDY OF NANO-INDENTATION. Ronald E. Miller, Dept of Mechanical and Aerospace Engineering, Carleton University, Ottawa, CANADA; Leo Shilkrot and W.A. Curtin, Division of Engineering, Brown University, Providence, RI.

We have developed a computational method to simultaneously model some regions of a material using discrete dislocation (DD) plasticity and others using a fully atomistic description. The CADD (coupled atomistic and discrete dislocations) method has been developed to study problems where it is expected that there are certain well-defined regions where atomistic effects will be important such as beneath an indenter or at grain boundaries. Although the method is currently limited to 2D, the approach expands our ability to bridge the length scales when modeling dislocation-mediated deformation phenomena. Existing discrete dislocation techniques correctly describe long-ranged elastic interactions between dislocations without the need for a fully atomistic description, but they cannot capture atomic scale interactions that are often essential for a full understanding of the behaviour. For example, dislocation nucleation, junction formation and annihilation are normally treated phenomenologically. Fully atomistic models, on the other hand, are limited to small system sizes relative to the size required to model microstructural features in real materials. CADD overcomes these difficulties by directly coupling a fully atomistic region to a finite-element based DD region. An important feature of the model is the ability to detect when it is energetically favourable for dislocations to move between the regions, and then automatically "convert" between the continuum and atomistic dislocation descriptions in a way that rigorously maintains compatibility across the atomistic/continuum interface. The phenomenon of nano-indentation by a spherical indenter into a thin film is simulated using the CADD method. The model allows us to identify the details of sub-surface, homogeneous dislocation nucleation in the atomistic region, and subsequent dislocation pile-ups at the film boundaries. These mechanisms can then be correlated with key features observed in experimental nano-indentation load-displacement curves. Finally, we have investigated the effects of pre-existing damage in the film by modeling multiple load-unload cycles.

2:30 PM W2.3
FRANK-READ SOURCES AND THEIR INTERACTION WITH GRAIN BOUNDARIES IN FCC ALUMINUM. Maurice de Koning, Wei Cai, and Vasily V. Bulatov, Lawrence Livermore National Laboratory, Livermore, CA.

We consider the operation of Frank-Read sources in FCC aluminum and their interactions with grain boundaries using a combination of atomistic and dislocation dynamics (DD) methods. The atomistic simulations show that a small Frank-Read source of a particular Burgers vector may, depending on the applied stress conditions, emit dislocations with a different Burgers vector in an indefinite (regenerative) sequence. In order to investigate whether this mechanism remains active for larger loop sizes we develop a mesoscale DD model of such source operation. The model is calibrated by matching its behavior to that of the atomistic model for a particular (small) loop size and involves a nucleation criterion for the formation of partial dislocation loops within an intrinsic stacking fault. We then use the calibrated DD model to extrapolate to the behavior of larger loops and obtain an estimate for the size interval within which the "unusual" mechanism seen in the atomistic simulations may be expected to remain operative. Finally, interactions of the source with two symmetric tilt grain boundaries will be discussed. 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.

2:45 PM W2.4
SPATIO-TEMPORAL PATTERNING IN MICROSCALE PLASTICITY. Masato Hiratani, Wei Cai, and Vasily V. Bulatov, Chemistry & Materials Science Directorate, Lawrence Livermore National Laboratory, Livermore, CA.

The self-organized criticality in plastic deformation is investigated by utilizing stochastic dislocation dynamics in nano-meso scale. Signal processing reveals both deterministic and chaotic behaviors of time series of plastic strain depending on loading conditions. The fractal behavior observed in short-time/small-scale simulations shows close resemblance to experimental data for long-time/ macroscale deformation instabilities i.e. Portevin-Le Chatelier effect whether local pinning obstacles are glissile or not. The existence of strange-attractors may reflect universal behavior of deformation patterning such as dislocation cells or walls. Similarity to dynamics of various topological defects in dissipative systems, bifurcation analysis by the effective field equations, and the associated intrinsic difficulties will be presented in this talk.

3:30 PM W2.5
DEVELOPMENT OF LARGE SCALE PARALLEL PARAMETRIC DISLOCATION DYNAMICS CODE WITH HIERARCHICAL TREE METHOD. Zhiqiang Wang, University of California, Dept of Aerospace and Mechanical Engineering, Los Angeles, CA; Sriram Swaminarayan, Los Alamos National Laboratory, Materials Science and Technology Division, MST-8, Los Alamos, NM; R. LeSar, Los Alamos National Laboratory, Theoretical Division, Los Alamos, NM; N.M. Ghoniem, University of California, Dept of Aerospace and Mechanical Engineering, Los Angeles, CA.

A parallel parametric dislocation dynamics code for 3D is developed with hierarchical representation of the computational domain. A hierarchical tree is constructed so that the domain is represented as the root node of the tree, the domain (root) is then recursively split to sub-domain (sub-nodes) until each leaf of the tree contain only a certain number of particles. Dislocations are distributed to different processors based on the distribution of sub-segments. Close-neighbors of dislocations are directly found by tree traversal. Far fields of dislocations are introduced using multipole expansion. Stress fields are expressed in Taylor expansions within a volume represented by hierarchical tree nodes. Large computational time scale from dislocation interaction can be decreased with this method.

3:45 PM W2.6
INTERNAL STRUCTURE OF A GEOMETRICALLY NECESSARY DISLOCATION BOUNDARY: DIRECT EXPERIMENTAL OBSERVATIONS AND INSIGHTS FROM ATOMISTIC MODELING. S.G. Srinivasan, R.J. McCabe, M.I. Baskes, A. Misra, and T.E. Mitchell, Los Alamos National Laboratory, MST-8 Structure/Property Relations, Los Alamos, NM.

Geometrically necessary dislocation boundaries (GNBs) are prevalent in deformation microstructures of medium to high stacking fault energy fcc metals. The orientation, spacing, and misorientaion relations of these structures are reasonably well understood. Not well understood are the internal dislocation structure of GNBs, their formation mechanisms, and the role these boundaries play in subsequent deformation. Detailed TEM studies of a GNB in rolled copper revealed a configuration consisting of dislocations from the two most highly stressed slip systems $[\bar{1}10](111)$ and $[101](\bar{1}11)$ and their sessile reaction product $[011](100)$ (Lomer lock). Atomistic simulations were used to gain insight into the formation and deformation behavior of this boundary structure. This work is supported by the U. S. Department of Energy, Office of Basic Energy Sciences.

4:00 PM W2.7
DISLOCATIONS AND STRENGTH IN SHOCKED Ta. James Cazamias and Dave Lassila, LLNL, Livermore, CA; Hussein Zbib, Washington State University, Pullman, WA.

Shock impact experiments have been performed to examine the strength of high purity [100] Ta in the dislocation drag regime. Samples have been recovered and TEM performed at various distances from the impact face to examine weak shock structure. VISAR experiments have been performed on .5 mm samples backed by sapphire to allow direct comparison with dislocation dynamics calculations. 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.

4:15 PM W2.8
CRYSTAL PLASTICITY BY LARGE SCALE DISLOCATION DYNAMICS. Wei Cai, Vasily V. Bulatov, Tim Pierce, Moono Rhee, Maria Bartelt and Meijie Tang, Lawrence Livermore National Laboratory, University of California, Livermore, CA.

Prediction of the plastic strength of single crystals based on the collective dynamics of dislocations has been a grand challenge for computational materials science for a number of years. The difficulty lies in the inability of the available dislocation dynamics (DD) codes

to handle a sufficiently large number of dislocation lines, in order to be statistically representative and to reproduce experimentally observed microstructures. Our new massively parallel DD code is capable of modeling million-dislocation systems by employing thousands of processors. We will discuss the methods that make simulations of such scale possible. Simulation data on stress-strain relationship, dislocation density and microstructure evolution will be presented and compared with experiments for FCC and BCC metals. We will discuss what sort of new information can be extracted from such simulations and examine how close we are able to come to understanding single crystal plasticity from the underlying collective motion of dislocations.

4:30 PM W2.9
DISLOCATION DYNAMICS VALIDATION EXPERIMENTS.
David H. Lassila, Mary LeBlanc, Tom Arsenlis and Moono Rhee, Lawrence Livermore National Laboratory, Livermore CA.

A unique "6-degree of freedom" (6DOF) deformation experiment has been fully developed specifically for the purpose of validation of dislocation dynamics simulations of plastic flow up to strains on the order of 1%. The experiment has been designed so that a compressive uniaxial stress field is essentially super imposed on the test sample, and the crystal is free to deform with 3 orthogonal translation directions, and 3 rotation/tilt axes of freedom. The rotation, tilt and translation of the crystal are monitored by 5 laser displacement gages and 3 extensometers. Experiments are being performed on high purity Mo single crystals orientated for "single slip". All of the experiments are performed in pairs, with one test sample having highly polished surfaces for optical light and AFM slip-trace analyses, and the other having 4 strain gage rosettes mounted on the sides for measurement of the bi-axial surface strains during testing. All of the experimental data is used together to determine the slip activity of the orientated single crystal during deformation. The experimentally observed slip activity during deformation can be correlated directly with that predicted by dislocation dynamics simulations that use realistic initial conditions (i.e., natural sources), thereby validating the simulation results.

4:45 PM W2.10
HIERARCHICAL CHARACTERIZATION OF DEFORMATION HETEROGENEITIES IN Mo SINGLE CRYSTAL. Erica Lilleodden and Nobumichi Tamura, Lawrence Berkeley Laboratory, Berkeley, CA; David Lassila, Lawrence Livermore National Laboratory, Livermore, CA; J.W. Morris, Jr., Lawrence Berkeley Laboratory, Berkeley, CA and Department of Materials Science and Engineering, University of California-Berkeley, Berkeley, CA.

Multiple length-scale characterization of Mo single-crystal after high strain rate compression loading has been carried out, providing a comprehensive picture of the deformation structure. Using a top down approach, optical microscopy, atomic force microscopy, x-ray microdiffraction and transmission electron microscopy have been used to identify regions of interest for finer-scale study. In this talk, we focus on results from microdiffraction experiments. High brilliance synchrotron sources used in conjunction with improved focusing optics have furthered the spatial resolution of x-ray diffraction measurements. A beamline at the Advanced Light Source (Lawrence Berkeley Laboratory) dedicated to microdiffraction experiments is used in scanning mode to map out Laue diffraction patterns across the surface of a sample, with a lateral resolution of 1 micron. These measurements have been analyzed in order to quantify the distribution of residual stress and strains in the sample, which in turn are related to the dislocation structure.

SESSION W3: DISLOCATION PHENOMENA AT THE ATOMISTIC LENGTH SCALE
Chairs: John A. Moriarty and Christopher Woodward
Wednesday Morning, April 23, 2003
Franciscan II/III (Argent)

8:30 AM *W3.1
FLEXIBLE FIRST-PRINCIPLES BOUNDARY CONDITIONS: SIMULATING ISOLATED DISLOCATIONS IN METALS.
C. Woodward, S.I. Rao, Air Force Research Laboratory, Wright Patterson AFB, OH.

First principles (FP) methods (e.g., electronic structure methods based on Density Functional Theory) provide a direct way of sampling how changes in chemistry influence materials properties. Recent improvements in numerical stability and parallel processing make FP simulations of several hundred atoms fairly routine. However, these are still very small simulation cells given the complexity of real alloy systems and the defects they contain. We offer a strategy for modeling defects in metals using informed boundary conditions, which are, derived from FP reference calculations. A flexible boundary condition method has been developed which can contain extended defects in very small simulation cells. Here the local strain field is self-consistently coupled to the long range elastic field using a lattice Greens Function method. This reduces the mesoscopic atomistic calculation to one only involving only the degrees of freedom near the defect center. As proof of concept FP methods have been used to evaluate the core structure and Peierls stress of isolated dislocations in BCC Mo, Ta and L10 TiAl. Predicted non-Schmid behavior in the BCC metals is consistent with experimental measurements. Also, the local strain field of the ordinary screw dislocation in TiAl gives insight as to the nature of the anomalous yield stress observed at high temperatures. These methods offer a clear path for directly evaluating solute-dislocation interactions and predicting solid solution strengthening.

9:00 AM *W3.2
STRUCTURE OF DISLOCATION CORES IN GaAs. S.P. Beckman, D.C. Chrzan, Materials Science and Engineering, University of California, Berkeley, CA and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA.

The structures of partial dislocation cores in GaAs are studied using an *ab initio* electronic structure total energy technique. Predicted structures of the α and β cores for both 30° and 90° partials are presented. For the case of the 90° partial dislocation, both the single and double period reconstructions are considered. These competing structures are found to be nearly degenerate in energy. This degeneracy suggests that, at temperature, both core reconstructions may be present. To explore this possibility, a simple statistical mechanical model for the competing core reconstructions is introduced. The model is used to study reconstruction domain sizes as a function of temperature. The implications for experimental determination of the structure of the 90° partial using high resolution electron microscopy are discussed. This work is supported by the Director, Office of Science, Office of Basic Energy Sciences, U.S. Department of Energy under contract No. DE-AC03-76SF00098.

9:30 AM W3.3
TEM IN SITU INVESTIGATION OF DISLOCATION BEHAVIOUR IN SEMICONDUCTORS AND THE INFLUENCE OF ELECTRONIC EXCITATION. Suzel Lavagne, Guy Vanderschaeve, Colette Levade, Daniel Caillard, CEMES CNRS, Toulouse, FRANCE.

TEM in situ straining experiments provide a unique way to investigate in real time the influence of various parameters (temperature, electron beam intensity, ...) on the behaviour of individual dislocations in semiconductors. Due to covalent bonding, dislocations experience a strong lattice friction: the experimental results are indeed consistent with a dislocation glide governed by the Peierls mechanism (i.e. nucleation and propagation of kink pairs), even for II-VI compounds which have a significant degree of ionic character. In III-V and II-VI compounds, a linear dependence of dislocation velocity with the length of the moving segment is noticed. Analysed in the framework of the kink diffusion model, this result indicates that dislocations move in the kink-collisionless regime. Kink formation and migration energies can be estimated from these experiments. For a variety of semiconductors the dislocation behaviour is sensitive to electronic excitations. A strong increase of dislocation mobility with increasing electron beam intensity is observed (radiation-enhanced dislocation glide). It is attributed to a lowering of the lattice friction, due to non-radiative recombinations of carriers at electronic levels associated with dislocations. In situ heating in the electron microscope makes it possible to study the dynamics of degradation defects induced by electron beam irradiation in ZnSe/GaAs heterostructures. Degradation occurs via the formation and propagation of conglomerations of dislocation loops in the active layer. This can be accounted for by a radiation-enhanced climb mechanism.

9:45 AM W3.4
THE RELEVANCE OF DISLOCATION CORE STRUCTURE TO KINK NUCLEATION IN $MoSi_2$. R.G. Hoagland, T.E. Mitchell, A. Misra, and M.I. Baskes, Los Alamos National Laboratory, Los Alamos, NM.

The species of dislocations that have been observed in bct $MoSi_2$ and related materials is extensive. Various Burgers vectors and slip planes are known to occur, but atomistic studies suggest that most are sessile, at least as straight dislocations. However, dislocation glide is most likely to proceed by nucleation and motion of kink pairs, and in $MoSi_2$, this must involve partial dislocations as the more relevant dislocations in this material dissociate into two or more components. Very recently, a model has been developed that describes the relation between kink nucleation rates and stacking fault energy, and, in so doing, enables a description of the basis for solid solution softening that has been experimentally observed. The model, which we describe, relies on linear elasticity for the energetics of double kink nucleation, but certain aspects of the problem must be assumed, e.g., the kink shape, or are uncertain, e.g., when the separation of partials is small.

Therefore, we also describe results of MEAM-based atomistic calculations that provide supplemental information for the model on kink energetics.

10:30 AM *W3.5
ROUGHENING TRANSITION IN SCREW DISLOCATION MOTION. Vasily V. Bulatov, Jaime Marian, and Wei Cai, Lawrence Livermore National Laboratory, University of California, Livermore, CA.

It is commonly assumed that Peierls stress delineates two different regimes of dislocation motion: (1) thermally activated motion by kink-pair mechanisms at stress below the Peierls stress and (2) phonon-drag controlled motion at stress above the Peierls threshold. We show, by means of large scale Molecular Dynamics simulations, that, instead of the expected transition at the Peierls stress, dislocation motion in BCC iron proceeds via previously unknown mechanisms that involve self-pinning and roughening of screw dislocations and produce a large number of debris loops in the wake of dislocation motion. Alternative to stress, transition from smooth to rough motion can be induced by changing the temperature or the length of screw dislocation lines. This strikingly unusual behavior can have serious implications for crystal strength, especially under high strain rate conditions.

11:00 AM W3.6
BYPASS OF A DISLOCATION NODE: EXPERIMENTAL OBSERVATIONS AND MODELING. R.J. McCabe, S.G. Srinivasan, and M.I. Baskes, Los Alamos National Laboratory, MST-8 Structure/Property Relations, Los Alamos, NM.

Dislocation nodes and networks are commonly seen in fcc deformation microstructures. They are believed to act as barriers to further dislocation motion and as key components of dislocation sources. Using in situ and stereo TEM, we find that a node observed in copper offers little resistance to a dislocation piled up at the node (one with the same Burgers vector and slip plane as one of the dislocations making the node). This behavior is further studied using atomistic simulations to gain insight into the bypass mechanism, and to determine the relative strength of the barrier. This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences.

11:15 AM W3.7
SIMULATING SHOCK PROPAGATION IN DEFECTIVE SINGLE CRYSTALS. E.M. Bringa, W. Cai, P. Erhart, N. Tanushev, M.J. Caturla, B.D. Wirth, and D. Kalantar, Lawrence Livermore National Laboratory, Livermore, CA.

Experimental samples in "single crystal" metals have an initial defect distribution that affects the plasticity threshold along the Hugoniot. In this work, shock propagation in single crystal Cu and Al is examined for different types of defect structures using molecular dynamics simulations. Changes in shock propagation due to voids were studied as a function of void size and shock pressure, giving a threshold pressure for collapse of a given void size. Shock propagation in nano-crystalline materials shows extra heating at the grain boundaries, leading to a reduced melting pressure. Finally, in order to account for possible dislocation sources, a prismatic loop that acted as a pair of Frank-Read sources was introduced, and the activation threshold for these sources was studied. These simulations are compared to Dislocation Dynamics simulations that include the role of partial dislocations, which is critical in the atomistic study. Connection to experiments that may detect the role of small defects in shock propagation will be discussed. 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.

11:30 AM W3.8
INFLUENCE OF 1/2a< 111 > SCREW DISLOCATION CORES ON DISLOCATION PROPERTIES IN BCC Ta. Guofeng Wang, Materials Science Division, Lawrence Berkeley National Laboratory, University of California, Berkeley, CA; Alejandro Strachan, Tahir Cagin, William A. Goddard III, Materials and Process Simulation Center, Beckman Institute, California Institute of Technology, Pasadena, CA.

For 1/2a< 111 > screw dislocations in bcc metals, two types of equilibrium core structures (symmetric core and asymmetric core) have been found from previous atomistic simulations. For an asymmetric (polarized) core, the central three atoms in the dislocation core would collectively translate along the Burgers vector direction causing a finite core polarization, while a symmetric (non-polarized) core has zero core polarization. Using a family of Embedded Atom Model (EAM) potentials all based on accurate Quantum Mechanics (QM) calculations, we investigated the relation between the properties of dislocation cores (core structure, core energy, core polarization, and core polarization curvature) and the dislocation properties (Peierls stresses and kink-pair formation energy) for 1/2a< 111 > screw dislocations in bcc Tantalum (Ta). In this work, we arrive at the following conclusions. (1) The equilibrium (non-polarized and polarized) dislocation core structures do not correspond to the Peierls stresses for those dislocations, (2) Instead, the Peierls stress correlates with the core polarization curvature around the equilibrium core configuration. The larger the core polarization curvature, the higher the calculated Peierls stress. (3) Both the equilibrium dislocation core structure and the core polarization curvature play important roles in determining the kink-pair formation energy. Keeping the core polarization curvature constant, the symmetric (non-polarized) core leads to lower kink-pair formation energy than the asymmetric (polarized) core. On the other hand, the kink-pair formation energy for a symmetric core increases with the increase of the core polarization curvature.

11:45 AM W3.9
ATOMISTIC AND DISLOCATION DYNAMICS SIMULATIONS OF PLASTIC HOMOLOGY IN BCC METALS UNDER PRESSURE. Lin H. Yang, Meijie Tang, and John A. Moriarty, Physics and Advanced Technologies Directorate, Lawrence Livermore National Laboratory, Livermore, CA.

At low temperature, the flow stress of bcc metals is controlled by the motion of (a/2)< 111 > screw dislocations. In turn, the mobility of these screw dislocations, is determined by the thermally activated formation and motion of kink pairs. In this work, we have performed detailed atomistic simulations of the kink-pair mechanism in the prototype bcc metals Ta and Mo at both ambient and high pressure, using quantum-based multi-ion interatomic potentials derived from model generalized pseudopotential theory (MGPT) together with Greens function flexible boundary conditions. Kink-pair activation enthalpies as a function of applied shear stress have thereby been calculated for pressures up to 2 Mbar. We then apply the pressure-dependent atomic-level data to study the homology of crystal plasticity in bcc metals by searching for a scaling relationship between the atomic-level flow stress and fundamental dislocation properties such as the Peierls stress and the kink-pair formation energy. Knowing such a scaling relationship also allows one to extend the prediction of plastic behavior to higher pressure, temperature and strain rate as well. Validation of the atomic-level plastic homology is obtained by performing corresponding 3D dislocation dynamics simulations using the atomic-level data as input.
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 number W-7405-ENG-48.

SESSION W4: MULTISCALE MODELING OF THIN FILMS AND NANO-INDENTATION
Chairs: Kevin J. Hemker and Erica Thea Lilleodden
Wednesday Afternoon, April 23, 2003
Franciscan II/III (Argent)

1:30 PM *W4.1
DISLOCATION FIELDS AND MOTION IN ANISOTROPIC AND MULTI-LAYER MATERIALS. Nasr M. Ghoniem and Xueli Han, School of Engineering and Applied Science, University of California, Los Angeles (UCLA), CA.

The motion of dislocations and their ensembles in anisotropic elastic materials is analyzed by an extension of the Parametric Dislocation Dynamics (PDD), originally developed for isotropic materials. The influence of elastic anisotropy on dislocation generation and hardening mechanisms will be discussed. In anisotropic multilayer thin films, typical of many emerging electronic and ultra-strong materials, a special technique is developed to deal with the effects of interfaces (i.e. image forces). Double Fourier transforms are used on the two coordinates within the thin film plane, while displacement and traction continuity are enforced at interfaces. Important features of the elastic field of parametric dislocation loops in these systems will be discussed. Several applications of these techniques in the simulation of material deformation will be given.

2:00 PM *W4.2
PLASTICITY RELATED PHENOMENA IN POLYCRISTALLINE METALLIC FILMS BONDED TO Si SUBSTRATES. Marc Legros, CEMES, Toulouse, FRANCE.

The strength of metallic films bonded to rigid substrate increases almost linearly with the inverse of their thickness. Constrained threading dislocation motion has been widely invoked to explain such dependence. On the other hand, the overall mechanical response of the film during thermal cycles can be better simulated using diffusion-based strain rate equations. The aim of this talk is to sort out the relative role of diffusion and dislocation processes in metallic

thin films using electron microscopy. Recent in situ experiments on metal films performed inside a TEM made possible the observation of dislocation motion during thermal cycles. Unexpected behaviors such as dislocation annihilation at the interface between the metal layer and the oxidized substrate were uncovered. In the case of Al on oxidized Si, the metallic film acts as a dislocation sink. This effect can only be slowed down by adding precipitates or a passivation layer. Results concerning bare or passivated Al and Au films, along with alloyed Al films will also be presented. It will be shown that the evolution of the film stress during thermal cycles can be qualitatively understood by combining in-situ and post-mortem TEM and SEM observations.

2:30 PM *W4.3
THREE DIMENSIONAL SIMULATION OF THE DISLOCATION DYNAMICS IN POLYCRYSTALLINE METAL THIN FILMS.
Burghard von Blanckenhagen, Universität Karlsruhe, Institut für Zuverlässigkeit von Bauteilen und Systemen; Eduard Arzt, Max-Planck-Institute for Metals Research, Stuttgart; Peter Gumbsch, Universität Karlsruhe, Institut für Zuverlässigkeit von Bauteilen und Systemen, and, Fraunhofer Institut für Werkstoffmechanik, Freiburg und Halle, GERMANY.

The plastic deformation of polycrystalline thin fcc metal films with thicknesses of one micron and less is investigated by using discrete dislocation simulations. The flow stress of polycrystalline thin films is much higher than for the corresponding bulk material and scales with the inverse film thickness. This effect is attributed to the dislocation motion in the confined geometry of the thin film. Experimentally this is well documented but theoretically not yet well understood. Furthermore, grain size and film thickness of these films are much smaller than the characteristic size of dislocation networks, which are observed in bulk material after deformation. The number of dislocations, which have to be considered in order to understand thin film plasticity, is strongly reduced. Therefore, discrete dislocation simulations offer themselves to investigate thin film deformation. Our simulations have shown that thin film models which consider the motion of dislocations extending over the entire film thickness either predict flow stresses much too small or cannot explain the scaling behavior. As a consequence, the activation of dislocation sources in thin films is investigated. This source model is thoroughly tested by calculating the response of randomly distributed dislocation sources to an applied stress and comparing the results with experimental data. Stress–strain curves, dislocation densities, work hardening rates and their dependence on the film thickness and grain orientation are investigated. The agreement between simulation and experiment is good and many aspects of thin film plasticity can be understood with the assumption that the deformation is controlled by the dislocation production and multiplication rather than the dislocation motion.

3:30 PM *W4.4
PARALLEL GLIDE: A FUNDAMENTALLY DIFFERENT TYPE OF DISLOCATION MOTION IN ULTRATHIN METAL FILMS.
T. John Balk, Gerhard Dehm and Eduard Arzt, Max-Planck-Institut fuer Metallforschung, Stuttgart, GERMANY.

When confronted by severe geometric constraints, dislocations may respond in unforeseen ways. This talk will present in-situ transmission electron microscope observations of parallel glide in unpassivated, ultrathin (200 nm and thinner) metal films, whereby dislocations glide parallel to and very near the film/substrate interface, following emission from grain boundaries. The biaxial film stress that evolves during thermal cycling should not drive such motion, and it is instead proposed that the observed dislocations are generated as a result of atomic diffusion into the grain boundaries. This provides experimental support for the Constrained Diffusional Creep model of Gao et al., in which they proposed that diffusional exchange of atoms between the unpassivated film surface and grain boundaries at high temperatures can locally relax the film stress near those boundaries. One feature of parallel glide at the nanoscale is that, as grain size decreases, eventually a single dislocation suffices to mediate plasticity in an entire grain during thermal cycling. This mechanism dominates the thermomechanical behavior of ultrathin, unpassivated copper films, and is a new example of the interactions between dislocations and the surface/interface. Such interactions are likely to increase in importance during the persistent miniaturization of thin film geometries.

4:00 PM W4.5
METALLIC ISLAND COALESCENCE: MOLECULAR DYNAMICS SIMULATIONS OF BOUNDARY FORMATION AND TENSILE STRAINS IN POLYCRYSTALLINE THIN FILMS.
A.R. Takahashi, C.V. Thompson, and W.C. Carter, Massachusetts Institute of Technology, Dept of Materials Science and Engineering, Cambridge, MA.

Island coalescence during the early stages of polycrystalline film formation is thought to lead to the large tensile stresses observed in experiments. Continuum models have been developed which are in semi-quantitative agreement with in-situ experimental observations of stress evolution during coalescence. However, the size of coalescing particles is in the nanometer range, so that atomistic treatments might be expected to more accurately reveal the mechanisms leading to coalescence stresses. We have performed molecular dynamics (MD) computational experiments in which small metallic clusters both in free space and on weakly bound substrates are allowed to coalesce. These atomistic simulations complement finite element modeling (FEM) and analytical work on the tensile strains developed during grain boundary formation by coalescence. Additionally, the atomistic simulations implicitly capture the effects of anisotropy and special orientations. The MD simulations also provide atomic-level detail of the boundary structure that is absent in continuum models. We have focused on simulations of Ag as a high mobility material at and above room temperature and have begun studying Ni as a material that can behave either as a high or low mobility material depending on the deposition temperature (i.e. Ni has a higher activation energy for adatom motion than Ag). We find that for small islands, the initial boundary formation occurs in times on the order of nanoseconds. For nanometer-sized clusters in free space and on traction-free substrates, the cluster can undergo large rotations prior to boundary formation. The MD simulated boundary lengths fit well with both FEM models and analytical models. The results of the simulations will be further quantified to relate the atomistic forces and positions to the stress state and we are pursuing methods for including the effects of traction at the interface, both through continuum and discrete methods.

4:15 PM W4.6
MULTI-SCALE CONTACT-INDUCED PLASTICITY IN Ni THIN FILMS: EXPERIMENTS AND MODELS.
J. Lou, Z. Zong, M. Huang, Princeton Univ, Princeton Materials Institute and Dept. of Mechanical and Aerospace Engineering, Princeton, NJ; A. Needleman, Brown Univ, Division of Engineering, Providence, RI; E. Vander Giesen, Univ. of Groningen, Dept. of Applied Physics, Groningen, THE NETHERLANDS; W.O. Soboyejo, Princeton Univ, Princeton Materials Institute and Dept. of Mechanical and Aerospace Engineering, Princeton, NJ.

This paper presents the results of a combined experimental and theoretical/numerical study of multi-scale contact-induced deformation in micro- and nano-scale thin films. Nanoindentation experiments are used to study the size dependence of hardness in single crystal Ni and polycrystalline LIGA Ni MEMS structures. The measured size effects and the observed dislocation pile-up phenomena are then explained using strain gradient plasticity theories and discrete dislocation models. Finally, a multi-scale framework is presented for the modeling of contact-induced deformation. This uses a combination of discrete dislocations and strain gradient plasticity theories to model contact-induced plastic deformation at the micro- and nano-scales.

4:30 PM W4.7
ATOMISTIC AND CONTINUUM STUDIES OF DIFFUSIONAL CREEP AND ASSOCIATED DISLOCATION MECHANISMS IN THIN FILMS ON SUBSTRATES.
M.J. Buehler, A. Hartmeier and H. Gao, Max Planck Institute for Metals Research, Stuttgart, GERMANY.

Recently developed theory of diffusional creep in metallic thin films constrained by substrates has identified a new class of defects called grain boundary diffusion wedges. These diffusion wedges are formed by stress driven mass transport between the free surface of the film and the grain boundaries during the process of substrate-constrained grain boundary diffusion. An important implication of the theoretical analysis is that dislocations with Burgers vector parallel to the interface can be nucleated at the root of the grain boundary. This is a new dislocation mechanism in thin films which contrasts to the well-known Mathews-Freund-Nix mechanism of threading dislocation propagation. Recent TEM experiments at the Max Planck Institute have shown that, while threading dislocations dominate in passivated metal films, parallel glide dislocations dominate in unpassivated copper films with thickness below 400nm. We have performed large-scale molecular dynamics (MD) simulations to model constrained diffusional creep and dislocation emission from cracked thin films. Nucleation of parallel glide dislocations competes with the classical threading dislocation mechanism and is coupled to diffusion activity. In MD simulations, we have observed nucleation of parallel glide dislocations from the root of the grain boundary, thus closing the theory-experiment-simulation linkage. We present a detailed atomistic analysis of constrained diffusional creep and subsequent dislocation nucleation process. Our atomistic modelling reveals that half planes of atoms are continuously inserted into the grain boundary leading to stress relaxation in the film. This pileup of climb dislocations can lead to a crack-like stress concentration at the interface of film and substrate, which may cause nucleation of dislocations with Burgers

vector parallel to the interface if the local dislocation density exceeds a threshold value. We will further present results regarding dislocation nucleation from cracks in thin films. The atomistic simulations support proposed theory as well as the experimental observations.

4:45 PM W4.8
SURFACE FILM ENHANCED PLASTICITY IN NIOBIUM OVER MULTIPLE LENGTH SCALES. C. Callamand, R. Gibala, University of Michigan, Ann Arbor, MI; V.K. Sethi, Western Research Institute, Laramie, WY.

We have examined the effect of surface oxide films on the mechanical behavior of niobium single crystal substrates involving two widely different length scales. Conventional macro-experiments have been performed in tension and compression on film-substrate composites involving 30-300 nm thick anodic oxide films deposited on 1-3 mm diameter crystals. These materials exhibit a pronounced decrease in yield and flow stresses and a substantial increase in plasticity relative to uncoated crystals when deformed at relatively low homologous temperatures and low strain rates. Similar crystals have also been deformed by nanoindentation techniques involving indentation depths of 30-3000 nm. At indentation depths below approximately 500 nm, the oxide-coated niobium is harder than the comparable uncoated material. At much larger indentation depths, 3000 nm and larger, the film-coated niobium is softer than the uncoated material, consistent with results in the macro-experiments. Models involving dislocation generation at the film-substrate interface and motion into the substrate are required to understand the combined behaviors.

SESSION W5: POSTER SESSION
MULTISCALE MODELING OF DISLOCATION PHENOMENA AND PLASTIC DEFORMATION
Chairs: Kevin J. Hemker, Lyle E. Levine and Hussein M. Zbib
Wednesday Evening, April 23, 2003
8:00 PM
Golden Gate (Marriott)

W5.1
ON THE INTERACTION BETWEEN Mg SOLUTE ATOMS AND DISLOCATIONS IN Al-Mg BINARY ALLOYS. Catalin Picu and Dawei Zhang, Dept of Mechanical Engineering, Rensselaer Polytechnic Institute, Troy, NY.

The interaction between solute atoms and dislocations is known to lead to negative strain rate sensitivity and poor formability. The negative rate sensitivity leads to inhomogeneous flow and the Portevin-LeChatelier effect. These observations motivate the present study of the solute-dislocation interaction in binary Al-Mg alloys. It is shown by means of atomistic simulations that Mg atoms form small clusters in Al in absence of any lattice defect. The clustering process is favored by a reduction in temperature and by tensile hydrostatic stress. Other stress components are seen to have a negligible effect on the clustering process. The diffusion mechanisms of Mg in bulk Al with and without vacancies is investigated and the barrier energies are computed. Pipe diffusion of Mg along the dislocation line is also investigated for dissociated dislocations. Finally, the Peierls stress required to move the dislocation in the solid solution is evaluated and compared with the threshold stress in pure Al.

W5.2
DISLOCATION CORE STRUCTURE DURING DISLOCATION GLIDE IN FCC AND BCC LATTICES. Catalin Picu and Monica Soare, Dept of Mechanical Engineering, Rensselaer Polytechnic Institute, Troy, NY.

A dislocation core model is developed in terms of a singular decomposition of the elastic field surrounding the dislocation in a power series of 1/rn. The decomposition is a Laurent expansion beginning with the terms corresponding to the Volterra dislocation and continuing with a series of dipoles and multipoles. The analysis is performed for both edge and screw dislocations in an fcc lattice and for screw dislocations in a bcc lattice. The field surrounding the dislocation is derived by means of atomistic simulations. The coefficients of the series expansion are determined from the elastic field using path independent integrals. When loaded by a shear stress smaller than the Peierls stress, the core distorts. The distortion up to the instability (Peierls stress) is monitored based on the variation of the coefficients. The differences between motion in fcc and bcc lattices and the pressure-shear coupling are discussed.

W5.3
SOME THEORETICAL ASPECTS OF THE GRÜNEISEN COEFFICIENT FOR THE EQUATION OF STATE OF SOLIDS. Francis Chaissé and Olivier Heuzé, CEA-DIF, Bruyeres-Le-Chatel, FRANCE.

The aim of this study is to specify the Grüneisen coefficient variation versus volume G(V). First, for isotropic solid, and in the harmonic approximation we recall the various classical laws on G(V). On the other hand, the shock wave physics have shown the experimental evidence of the linear relationship between shock velocity (U) versus jump of particle velocity (u) with some further consequences on G(V) [cf. MRS Symp. Proc. vol 731 paper W81 (Spring 2002)]. In this paper, we point out the failure of the G(V) representation in the harmonic approximation to reproduce the shock wave data U(u). Taking now into account the anharmonic effects in solids, we propound a new analysis of the G(V) law which is well suited for the shock wave physics of solids.

W5.4
ELASTIC PROPERTIES OF POLYCRYSTALS. Rajeev Ahluwalia, Turab Lookman, Avadh Saxena, Theoretical Division, Los Alamos National Lab, NM.

We propose a framework based on Ginzburg-Landau theory to model the elastic properties of polycrystals. In this approach, elastic strains are coupled to an orientational field describing the crystallites. The orientational field is determined from a phase field model of grain growth. We apply this model to simulate mechanical properties of linear elastic materials as well as shape memory materials that are governed by nonlinear effects.

W5.5
A COMBINED AB-INITIO AND BOND-ORDER POTENTIALS STUDY OF COHESION IN IRIDIUM. M.J. Cawkwell[a], D. Nguyen-Manh[b], V. Vitek[a] and D.G. Pettifor[b]. [a]Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA; [b]Department of Materials, University of Oxford, Oxford, UNITED KINGDOM.

Given its high melting temperature and excellent oxidation and corrosion resistance, iridium might form the basis for a family of refractory intermetallics. Yet, pure iridium exhibits mechanical and physical properties that are substantially different from those of other materials crystallizing in the face–centered–cubic (fcc) structure. Most notably, iridium is the only fcc metal that cleaves in the single crystal form even at room temperature. Moreover, its elastic moduli are unusual in that the Cauchy pressure ($C_{12} - C_{44}$) is negative and [k, k, 0] phonon branch is anomalous. These deviations from the norm of fcc materials suggest a strong non–central interatomic bonding that combines with the metallic bonding, as is common in compounds such as transition metal silicides. Consequently, while in most fcc metals atomic interactions can be treated with sufficient accuracy in the framework of many–body central–force methods, such as EAM or Finnis–Sinclair type potentials, this approach is not applicable in iridium. For this reason, we first investigate the cohesive properties of iridium using *ab–initio* FP–LAPW methods and develop a Bond–Order Potential (BOP), a tight–binding formalism that is able to describe materials with mixed covalent and metallic bonding through physically transparent parameterizations. The constructed BOP is then tested by its ability to reproduce vacancy formation energies and phonon spectra that have been determined experimentally, along with structural energy differences, deformation paths and stacking fault energies calculated *ab–initio*. Such a description of atomic interations is then suitable for more complex atomistic studies of the structure and properties of defects governing mechanical behavior, in particular dislocations and grain boundaries. This research was supported in part (MJC and VV) by the U.S. Department of Energy, BES Grant. no. DE-FG02-98ER45702.

W5.6
Abstract Withdrawn.

W5.7
MESOSCALE DISLOCATION PATTERNING AT FINITE CRYSTAL DEFORMATION. Anter El-Azab, Fundamental Science Directorate, Pacific Northwest National Laboratory, Richland, WA; Michael Zaiser, Center for Materials Science and Engineering, University of Edinburgh, Edinburgh, UNITED KINGDOM.

Plastic distortion of metals is characterized by complex dislocation dynamics and interactions giving rise to a rich variety of mesoscale dislocation structures. The evolution of structures are important in a number of respects, such as strain localization and plastic instabilities, development of constitutive response models, and in understanding the interaction between the alloy microchemistry and deformation-induced structures. A statistical approach to the dynamics of large dislocation systems at finite crystal distortions will be discussed. In this approach, we invoke the mathematics of stochastic fiber processes to develop kinetic equations governing the transport, reactions and multiplication of dislocations. The dislocation system is viewed as a statistical system of linear entities whose

interactions are mediated by the crystal elasticity. Adopting the Klimontovich's kinetic theory view as a starting point, the analogues of the n-particle correlations are developed for the dislocation system. Hierarchies of the kinetic equations up to second order are then developed in both the deformed and reference configurations of the crystal, along with a set of gauge constraints that must be satisfied by these equations. In doing so, the overall dislocation population is split into multiple statistical systems that overlap in the crystal space. In order to demonstrate the power of this approach in providing a systematic way of coarse-graining of dislocation systems, we extract specialized model for straight edge dislocations and solve the pertinent equations for the evolution of the dislocation distribution and other distortion and elastic fields. Particular attention is given to the importance of lattice rotation and dislocation-dislocation correlation.

W5.8
MULTISCALE MODELING OF BRITTLE TO DUCTILE TRANSITIONS. S.J. Noronha and N.M. Ghoniem, University of California-Los Angeles, Department of Mechanical and Aerospace Engineering, Los Angeles, CA.

We implement a multiscale approach in which Finite element method (FEM) is directly coupled to Dislocation dynamics (DD) simulations. The DD simulations in turn use parameters obtained by atomistic simulation. We study the brittle to ductile transition behavior of ferritic steels, where micro-cracks triggered by secondary particles are detrimental. The four-point bend tests were simulated with FEM-DD approach to study the microstructural details. The statistical nature of the experimental data are simulated are compared.

W5.9
MULTISCALE STUDY OF SELF-INTERSTITIAL DUFFUSION IN VANADIUM. Luis A. Zepeda-Ruiz, Lawrence Livermore National Laboratory, MSTD/CMS, Livermore, CA; Seungwu Han, Roberto Car, David J. Srolovitz, Princeton Materials Institute, Princeton University, Princeton, NJ; Graeme J. Ackland, Dept. of Physics and Astronomy, University of Edinburgh, Edinburgh, Scotland, UNITED KINGDOM.

Self-interstitial atoms (SIA) produced during collision cascades are key components of the microstructure observed when metals are irradiated with high-energy particles. These interstitials play a key role in determining the mechanical properties of irradiated metals. Knowledge of the formation and diffusion mechanisms of SIA is essential for understanding and predicting the effects of radiation damage. In the present study, the fundamental point defect (vacancy, tetrahedral and octahedral interstitials, $< 111 >$ crowdion, and $< 111 >$, $< 110 >$, and $< 100 >$ split interstitials) properties (formation energies and migration barriers) are first determined using first principles methods. Based on this information a new interatomic potential for vanadium is developed and used in molecular dynamics simulations (MD) to study the diffusion mechanisms of SIA in V. Results show that the SIA in vanadium exists in a $< 111 >$-dumbell configuration and migrates quickly along $< 111 >$ directions, even at very low temperatures. Rotation of the dumbbells and the migration path to other $< 111 >$ occurs with increasing frequency as the temperature is raised. It was found that the apparent activation energy for diffusion increases with increasing temperature. This increase in apparent activation energy with increasing temperature occurs even at temperatures that are too low to be attributed to dumbbell rotation. Rather, we demonstrate that the intrinsic activation energy is not strongly temperature dependent, but rather the correlation factor is. A simple physical model for this effect is proposed. Detailed comparisons of the simulation results with experimental measurements of diffusivity and interstitial structure will be presented.

W5.10
DISLOCATION DYNAMICS SIMULATIONS OF DISLOCATION STRUCTURE REARRANGEMENT IN COPPER SINGLE CRYSTAL UNDER MULTI-STEP CYCLIC LOADING. Miaolin Feng, Jixi Zhang, Yanyao Jiang, Department of Mechanical Engineering (312) University of Nevada, Reno, NV.

A copper single crystal subjected to cyclic loading displays in the cyclic stress-strain curve three distinct regions characterized with unique dislocation structure configurations. Experimental observations on the copper subjected to high-low two-step sequence loading revealed that the cell and labyrinth structures produced by the high amplitude loading can be rearranged to the persistent slip band (PSB) ladder structure in the subsequent low amplitude loading within the plateau region of cyclic stress-strain curve. The ladder structure started to form in the early stages during the second-step loading and the dislocation wall spacing of the ladder structure gradually increased with increasing accumulation of plastic deformation. Based on the theories of Needleman, a two-dimensional (2D) dislocation dynamics model was developed considering the dislocations generated from the Frank-Read source and the interaction among the dislocations. The formation of the dislocation structure configurations associated with the three distinctive regions in the cyclic stress-strain curve of a copper single crystal was successfully simulated. Furthermore, the evolution of the dislocation structures of the material subjected to the high-low two-step loading sequence was simulated with results in favorable agreement with the experimental observations. Discussions were made on the advantages and disadvantages in using a 2D dislocation dynamics model.

W5.11
A SESSILE DISLOCATION ARRANGEMENT IN ZrN. Peng Li, James Howe.

Dissociation of perfect 1/2<110> single dislocations into two 1/6<112> Shockley partial dislocations in ZrN phase was observed in the transmission electron microscope (TEM). The 1/2<110> single dislocations have a super-jog character and are not coplanar with the dissociated Shockley partials. This sessile arrangement of dislocations may be responsible for the brittleness of ZrN. The wide separation of the partial dislocations bounding the stacking faults indicates that the stacking faults energy (SFE) in ZrN is low. This unusually low SFE can be explained on the basis of a high vacancy concentration in ZrN, which was confirmed by the appearance of diffuse intensity maxima in electron diffraction patterns due to short-range ordering of N vacancies. In-situ heating experiments in the TEM revealed that the diffuse intensity maxima disappear during heating. This indicates that the vacancy concentration in ZrN increases during heating. The width of the two partial dislocations increases with temperature, as the SFE changes with the vacancy concentration.

W5.12
THE PLASTICALLY DEFORMED ZONE SURROUNDING VOIDS IN SINGLE CRYSTAL ALUMINUM FROM INCIPIENT SPALLATION FRACTURE EXPERIMENTS. James Belak, James Cazamias, Marc Fivel†, David Haupt, John Kinney, Mukul Kumar, Roger Minich, Robert E. Rudd, Eira T. Seppälä, and Adam Schwartz, Lawrence Livermore National Laboratory, Livermore, CA; †GPM2 CNRS/INPG, Domaine Universitaire, Grenoble, FRANCE.

The dynamic fracture of ductile metals is known to occur through the nucleation and growth of microscopic voids. As the voids grow, the surrounding metal is plastically deformed to accommodate the change in void volume. Despite this qualitative understanding, little direct experimental evidence is available concerning the details of this plastically deformed zone for high rate experiments, in particular the evolving dislocation structure. In order to gain better insight into this plastically deformed zone, we performed a series of incipient spallation fracture experiments on single crystal aluminum shocked in the [001], [011], [111], and [123] directions. Concurrently during the soft recovery experiment, the in situ free surface velocity wave profile was measured. The wave profile gives details of the stress transient to which the sample was subjected. Prior to metallurgical analysis, the void size and spatial distribution were determined directly from X-ray tomography. The plastically damaged zone surrounding the voids was initially revealed during the etching to produce samples for electron backscattering microscopy. The EBS data gives direct information on the local rotation of the crystal lattice in the plastic zone. Nanoindentation was used to measure the microhardness in the plastic zone. The measurements indicate this region to be harder than the surrounding metal. The size of the zone was consistent between the three experiments. TEM was then used to measure the dislocation structures inside the plastically damaged zone. Acknowledgment: This work was performed under the auspices of the US Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

W5.13
MODELLING OF MOLECULAR PROCESSES IN CREEP OFAMORPHOUS-CRYSTALLINE POLYMER. Ulmas Gafurov, Institute of Nuclear Physics, Tashkent, Ulugbek, UZBEKISTAN.

The molecular models chain slippage and chain rupture of interconnecting macromolecules for an oriented loaded semi-crystalline polymer and complex interaction between slippage and rupture of polymer chains using Frenkel-Kontorova's dislocation models has been suggested. The polymer was considered as two-phase one with interchanging amorphous and crystalline regions After some polymer elastic stretching and conformation straightening of an interconnecting chain the consecutive slippage of one followed with thermo-fluctuation formation of a dislocation in polymer crystalline regions. The dislocation movement into crystallite and accordingly the further slippage of the passage macromolecule fastened by cross-link happens with increase of local load on crystallite boundary and with enhance of dislocation energy. While for the interconnecting macromolecules without cross-linking the slippage is accompanied by loss of the kink energy. We consider conditions under which

thermo-fluctuation rupture of a chemical bond of a stretched linear atomic macromolecular chain takes place. In the case non-fixed (or fixed only intermolecular bonds) increasing of the local load on the chain leads to the new act of slippage. So, such non-fixed macromolecule could not be ruptured. The favorable condition to chain rupture are formed for stressed section of macromolecule fixed on polymer crystallite surface or in entanglements.

W5.14
ANISOTROPY OF NANOINDENTATION - A TOOL FOR THE DETERMINATION OF NANOCRYSTAL ORIENTATION? David Christopher, Roger Smith and Steven Kenny, School of Mathematics and Physics, Loughborough University, Loughborough, UNITED KINGDOM; Bodo Wolf and Asta Richter, Department of Engineering Physics, University of Applied Sciences Wildau, GERMANY.

The paper presents a novel look at nanoindentation patterns in crystalline materials and shows how the piling up of material, reflected in the shape of the topography around the indentation hole, can be used as a tool to investigate structure. If nanoindentation is combined with surface imaging not only can the nanomechanical properties be tested but the pattern around the indentation hole gives clues about the crystalline orientation. Nanoindentation into ionic crystals (SrTiO3), covalently bonded semiconductors (GaAs and In0.53Ga0.47As) and metals (Fe) were performed, the latter being combined with classical molecular dynamics (MD) simulations on the Fe(100), Fe(110) and Fe(111) surfaces. For the Fe(110) surface the indentation pattern for a spherocone shows two symmetric pile-ups orientated along the $< 100 >$ surface direction. When a cube corner indenter is used then the pattern changes as the crystal is rotated. If a side of the indenter is aligned with its normal along this $< 100 >$ direction a large pile up occurs along this side. The indentation pattern shows a complex combination of the indenter geometry with the underlying crystal symmetry which is explained through the use of large scale MD simulations (> 1.2 million atoms) and computer movies. These show how dislocation loops generate from the tip and for the (110) surface carry material away from the hole. There is excellent agreement between the simulations and experiment for all low index surfaces. In the case of SrTiO3, the imprints are accompanied by formation of slip bands. The GaAs(100) surface possesses a fourfold inversion symmetry axis, and the piling up structure was also found to exhibit fourfold symmetry. The new technique will be especially useful for textured materials where the surface orientation is generally known but there are domains which are rotated around the surface normal. However it can also be used to investigate homogeneous materials where the surface orientation itself is not known.

W5.15
Abstract Withdrawn.

W5.16
PLASTIC RELAXATION IN HETEROEPITAXIAL METALLIC THIN FILMS. Sébastien Groh, Ladislas Kubin and Benoit Devincre, LEM, UMR104 CNRS-ONERA, Chatillon, FRANCE.

The growth of a thin epitaxial film on a substrate of different nature induces internal stresses in the film. These stresses are uniform and depend on the mismatch strain between the two lattices. Beyond a certain critical thickness, the total elastic energy of the film can be relaxed by misfit dislocations that appear at the film-substrate interface. The classical model by Matthews, which is formulated within the framework of isotropic elasticity, predicts a lower bound for this critical thickness value. The reasons why plastic relaxation is more difficult than expected have, therefore, been the object of some discussions. The objective of the present work is to compute internal stresses in epitaxial layers in a rigorous manner, in particular by accounting for the influence of elastic anisotropy. Results on the influence of several parameters which govern the plastic relaxation, such as the film thickness, the local line tension of the dislocation, the elastic anisotropy of the film and the substrate and the orientation of the film are presented and discussed. These results were obtained with the help of an hybrid simulation method, the discrete-continuum model. In this model, a simulation of dislocation dynamics is coupled to a finite element code which solves the boundary value problem. Numerical simulations conducted on model Cu/Cu, Cu/Ag and Cu/Ni systems with a (001) orientation show that all the parameters listed above induce a significant increase of the critical thickness in comparison with the values predicted by the Matthews model. Finally a comparison of the anisotropic critical thickness between (001) and (111) interfaces shows that (111) copper films are about twice harder than (001) films. It is thus concluded, that elastic anisotropy effects and may explain at least partly the observed discrepancies between the predictions of classical isotropic models and experimental observations.

W5.17
SUPER HARDNENING OF W/NbN NANOLAYERS UNDER SHALLOW NANOINDENTATION. B.M. Ennis, W.S. Slaughter, S.X. Mao, Dept. of Mechanical Engineering, University of Pittsburgh, Pittsburgh, PA.

Superlattice materials are nanocomposites that exhibit a hardness at small bilayer repeat periods which exceeds the hardness predicted by the rule of mixtures for normal composites. The objective of this investigation was to utilize the experimental data obtained from nanoindentations and image scanning to examine the behavior of the superlattice material, W/NbN. Nanoindentations and in situ surface imaging were conducted over a range of applied loads on samples of W/NbN with two different bilayer periods ($=5.6$ nm and $=10.4$ nm), and monolithic samples of the niobium nitride (NbN) ceramic and the tungsten (W) metal which comprise the superlattice material. Additional shallow nanoindentations were made to a depth equal to the individual layer thicknesses of the nanocomposites. The mechanical properties were determined using the Oliver and Pharr method and compared for all the samples. The load versus displacement curves are also compared. The energies of indentation are calculated. The characteristics of the material pile-up resulting from the nanoindentations are determined from the scanned surface images. The experimental results are discussed to evaluate the influence of the different factors to the observed increase in hardness. The results indicate that the elastic modulus does not influence the hardness of the superlattice materials. The hardness and load versus displacement curves for the shallow indentations show little difference in behavior between the NbN sample and the two superlattice materials. However, an increase in hardness is observed in the superlattice materials at deeper indentation depths. The results indicate that this increase in hardness is related to the nature of the interface between the layers in the superlattice materials.

W5.18
FEATURES OF SEMICONDUCTORS DURING NANOINDENTATION. Asta Richter and Bodo Wolf, University of Applied Sciences, Wildau, GERMANY; and Roger Smith, Loughborough University, UNITED KINGDOM.

The paper presents novel features of semiconducting materials with nanoindentation which is a new technique for investigation of mechanical properties on nanoscale. The experiments are performed in a modified scanning force microscope (SFM) which allows to measure the force and the corresponding penetration depth simultaneously. Different diamond indenters with various shapes are used for penetration into the material up to forces of 6 mN. After indentation the same tip can be used to image the surface within the SFM mode. Multicycling experiments with intelligent load-time functions of several segments are used to obtain more information on the materials properties than the standard values such as the hardness and the indentation modulus. The differential hardness registers local hardness values in dependence on the depth. The changes in hardness with depth reflect several deformation states and are a measure of properties either induced in the material by the contact pressure of the tip during indentation and/or the inherent mechanical properties of the material. Reloading after partial unloading is an excellent indicator for inelastic processes that become visible by hysteresis loop formation. These loops can be due to sample viscosity as for many polymers, but can be also correlated with phase transformations in semiconducting materials. The phase transitions in InSb and Si depend on the value of the implantation dose and the amorphisation of the material. Beside features in the force-depth curve, the image of the imprint reflects also the crystalline structure of the material with characteristic pattern of the topography around the indentation hole which are representative for the crystallographic orientation. Molecular dynamics simulations have been carried out to study the mechanisms on atomic scale which result in the generation of defects such as dislocations, dislocation loops, slip bands and materials transport away from the indentation hole.

W5.19
MATERIAL LENGTH SCALE CONTROLLED STRAIN GRADIENT SENSITIVITY IN METALLIC SINGLE CRYSTALS. Scott Mao, Minhua Zhao, W.S. Slaughter, University of Pittsburgh, Dept of Mechanical Engineering, Pittsburgh, PA.

This paper correlates the experimental results of indentation size effect with the predictions from a non uniform strain gradient plasticity indentation model. Nanoindentations on single crystal of Al, Ag, Ni and annealed large grain size Cu, PST lamellar α_2-TiAl and γ-TiAl are conducted by AFM/Hysitron nanoindenter. Nanoindentaion hardness is normalized by the hardness at 1000nm depth of indentation, which is used to compare the indentation size effect of different materials. It's been found that there exists a characteristic material length scale, which is a function of burgers vector, shear modulus and reference stress of the materials, controls

the size effect in nanoindentation. The material length scale is in the order of $l_{m,Ag} > l_{m,Ni} > l_{m,Al} > l_{m,Cu} > l_{m,\alpha_2 TiAl} > l_{m,\gamma TiAl}$, while the same is true for the indentation size effect of those materials. Furthermore, parameters involved in the non uniform strain gradient model, such as material length scale, reference stress and stress-strain index, can also be derived from micro indentation test. The predictions of indentation size effect from non uniform strain gradient plasticity model are compared with the nanoindentation results. It is revealed that predictions fit reasonably with the nanoindentation results using the parameters from micro indentations.

W5.20
PLASTICITY IN POLYCRYSTALLINE THIN FILMS: A 2D DISLOCATION DYNAMICS APPROACH. Lucia Nicola and Erik Van der Giessen, University of Groningen-Netherlands Institute for Metals Research, Groningen, THE NETHERLANDS; Alan Needleman, Brown University, Providence, RI.

Stress relaxation in thin films is analyzed by mean of discrete dislocation simulations. While cooling from a stress free configuration, stress builds up in the film due to thermal mismatch with the infinitely large substrate to which it is perfectly bonded. The film is modeled as a periodic repetition of a few columnar grains, containing three slip systems each. Dislocations can be generated and glide on the slip planes according to constitutive rules. The coating-substrate interface as well as the grain boundaries are treated as impenetrable barriers for the dislocations. The substrate behaves elastically during the whole simulation while the stress in the film gets partly relaxed by dislocations glide. The evolution of the stress state in the film is calculated at each time increment accounting for dislocation dynamics. This is done by coupling the analytic infinite medium solution for the discrete dislocations in the film to the numerical solution of a boundary value problem. The objective of these simulations is to gain insight into the dependence of film hardening on thickness and grain size.

W5.21
Abstract Withdrawn.

W5.22
DISLOCATION DYNAMICS SIMULATIONS OF PLASTIC DEFORMATION IN BCC THIN FOILS. Meijie Tang, Physics and Advanced Technology Directorate, Lawrence Livermore National Laboratory, Livermore, CA; Guanshui Xu, Dept. of Mechanical Engineering, Univ. of California, Riverside, CA.

Early experiments showed that the plastic deformation (yield behavior) of bcc single crystal thin foils were strongly influenced by surface orientation and temperature[D. Vesely, Scripta Metal., 6, 753 (1972)]. This was interpreted mainly based on the low mobility of screw dislocations at low temperatures. We developed a dislocation dynamics simulation method[M. Tang, L. P. Kubin, G. R. Canova, Acta Mater. 46, 3221 (1998)] coupled with a finite element method to study this problem. The FEM is used to deal with boundary effects due to free surfaces. Simulations are performed in detail to investigate the surface orientation, foil thickness, and temperature dependence of the bcc plastic behavior. Results will be presented for single crystal Tantalum. The work of Meijie Tang is performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

W5.23
THE MECHANISM OF MISFIT STRAIN RELAXATION IN EPITAXIALLY GROWN BLT($Bi_{4-x}La_xTi_3O_{12}$) THIN FILMS. Hyung Seok Kim, Ju Hyung Suh, Sang Ho Oh, and Chan Gyung Park, Pohang University of Science and Technology, POSTECH, Dept of Material Science & Engineering, Pohang, KOREA.

Layered perovskite structured lantanium bismuth titanate, $Bi_{4-x}La_xTi_3O_{12}$ (x≈0.75, BLT) is a candidate material for FRAM (Ferroelectric Random Access Memory) capacitor. When the BLT thin film is grown epitaxially, the lattice mismatch between BLT and substrate can affect the electrical characteristics. Therefore, understanding the relaxation of misfit strain in epitaxially grown BLT thin films is very important. However, only a few studies has been reported on the mechanism of misfit strain relaxation in layered perovskite materials. In the present work, relaxation of misfit strain in BLT films has been investigated by transmission electron microscopy (TEM). R.F. magnetron sputtering was employed to grow BLT thin films on $SrTiO_3$ (STO) and $LaAlO_3$ (LAO) substrates at 700°C. The thicknesses of deposited films were 20 nm and 100 nm because density of misfit dislocation increased and saturated at those thicknesses. Since lattice parameters of BLT $1/2\,a_{110}$ (0.3854 nm), STO a_{100} (0.3939 nm) and LAO a_{100} (0.3846 nm) are very similar at 700°C, $1/2\,a_{110}$ of BLT unit cell corresponded to the a_{100} of the two substrates. Thus, tensile strain (-2.03%) was induced to the BLT grown on STO and compressive strain (+0.201%) was applied to the BLT on LAO during the growth. When BLT thin film was deposited on STO, misfit strain was relaxed by the formation of misfit dislocations at 20 nm thickness and by the formation of crack at 100 nm. Bugers vector of misfit dislocations was $a_{asubstrate,100}$ and direction of crack was $[100]_{substrate}$ or $[010]_{substrate}$. In the case of BLT grown on LAO, the magnitude of lattice misfit between BLT thin film and LAO substrate is small (~1/10) in comparison with that of BLT/STO. Misfit dislocations or cracks were not observed up to 100 nm thickness. But compressive stress resulted in the distortion of atomic layers and the formation of mis-orientation regions.

W5.24
ADATOM-SUBSTRATE ELASTIC INTERACTIONS: IN-SITU EXPERIMENTS, EMBEDDED ATOM SIMULATIONS, AND DENSITY FUNCTIONAL THEORY CALCULATIONS.
Cody Friesen, Carl V. Thompson, and Nicola Marzari, Massachusetts Institute of Technology, Cambridge, MA.

A fundamental aspect of the growth of thin films is the adsorption of atoms onto the film surface. The long range elastic interaction between the adatoms and the surface plays a large role in the subsequent elementary processes of film growth, such as diffusion, clustering, and adsorption at step and kink sites. The quantity that specifies the strength of the interaction, as treated analytically employing the elastic Green's function for a half space, is the force-dipole tensor A_{ij}. In this study, highly sensitive real-time in-situ stress measurements were performed in an ultra high vacuum environment, allowing the extraction of the force-dipole magnitude as a function of temperature for the adatom-substrate interaction for both homo- and hetero-adatoms. The systems studied experimentally thus far are < 111 > textured face-centered cubic metallic surfaces with metallic adatoms. We have examined the homo-adatom systems Cu, Au, and Ag and the hetero-adatom systems Cu/Au (adatom/surface) and Au/Cu. To determine the temperature dependence of the interaction, embedded atom method (EAM) simulations were performed for the Cu/Cu and Ag/Ag systems on both the (111) and (001) surfaces. Furthermore, density functional theory (DFT) based calculations have been employed to obtain accurate force-dipole magnitudes for both homo- and hetero-adatoms for several of the experimental systems. This problem is intrinsically multiscale in that experiments yield force-dipole magnitudes that are most easily analyzed through mesoscale theory (elasticity), but in order to determine the specific magnitude of the force-dipoles in different systems, the problem must be treated quantum mechanically and analysis of the dependence of the adatom-substrate interactions on variations in density and temperature is only possible through the use of classical many-body interatomic potentials.

W5.25
STRAIN RELAXATION BY MISFIT DISLOCATION ARRAYS. Prita Pant and Shefford P. Baker, Department of Materials Science and Engineering, Cornell University, Ithaca, NY.

Several models have been proposed for the strain relaxation of thin FCC films by the formation of misfit dislocations of mixed character. However none of these models take into account the shear strains introduced in the film by the misfit dislocations. An analytical model for the strain relaxation of thin films by misfit dislocation arrays is presented that takes into account all components of the strain tensor, including shear strains. The model is applied to strain relaxation in (001), (111), and (011) oriented FCC metal films. Our results show that shear strains strongly influence the total strain energy of the film. Since both the critical strain for dislocation formation, and the equilibrium spacing of dislocations in arrays depend on the minimum energy values, these quantities are found to be different from those predicted by previous models. It is also shown that the residual stresses in a film may be quite different depending on the combination of arrays formed during relaxation. These results may aid in understanding the inhomogeneous stress states experimentally observed in films under uniform biaxial applied strain.

W5.26
INHOMOGENEOUS DISTRIBUTION OF DISLOCATION DENSITY AS MANIFESTATION OF MULTISCALE STRUCTURE IN TUBES FROM Zr-BASED ALLOYS. Margarita Isaenkova and Yuriy Perlovich, Moscow Engineering Physics Inst, Dept of Physical Problems of Materials Science, Moscow, RUSSIA.

An X-ray method was developed to determine the dislocation density in metal materials as a distribution depending on the orientation of Burgers vector. The method includes registration of X-ray line profiles by each successive position of the sample in the course of diffractometric texture measurement using reflections of two orders, the following determination of coherent domain size and lattice distortion by means of the Warren method for each orientation of reflecting planes, separate calculation of the density of dislocations

with all possible orientations of Burgers vector and presentation of obtained results in the generalized pole figure. The method was used to determine the dislocation density in tubes of Zr-based alloys for nuclear industry, consisting mainly of α-Zr phase with HCP crystalline lattice. Distributions of c- and a-dislocations were constructed as generalized pole figures and, by use of usual texture pole figures, they were recalculated into distributions of grain volume fractions with different dislocation densities. Obtained data show, that the dislocation density varies within very wide interval of several orders of magnitude depending on the grain orientation: from 10^{12} to 10^{17} m^{-2} in the as-rolled tube and to 10^{16} m^{-2} in the same tube after polygonization annealing. The density of c-dislocations in α-Zr grains grows as their basal axes move away from the transversal section of tube. Though, according to the conventional conception, the found maximal values of dislocation density seem to be raised too high, the revealed tendency is undoubted: any portion of deformed metal of several cubic mm in volume contains a continuous series of fractions with increasing dislocation densities, so that within some regions the lattice distortion attains its limit. At the same time, in the orientational space these regions are distinctly localized within texture minima. By analysis of mechanical and radiation behavior of tubes it is necessary to consider them as composites.

W5.27

DISLOCATION AND GRAIN DERIVED THEORY OF DESCRIPTIVE KINEMATIC METRICS OF FINITE DEFORMATION TO REPLACE EXISTING ELASTIC-PLASTIC PHENOMENOLOGICAL METRICS. Ray B. Stout, University of California/LLNL, Livermore, CA.

Existing kinematic metrics used for correlating experimental data sets from finite deformation tests are traceable to a two reference state, deformed elastic-plastic back to an idealized zero stress plastic state, configuration analyses proposed primarily by E.H. Lee (Lee, 1970). These analyses admit that material discontinuities would exist in arriving at a virtual state of the zero residual stress, however, the elastic-plastic deformation process is considered a mathematically continuous spatial function process. Hence, no length scale metrics are analytically introduced because of the continuity requirements of the embedded deformation function space. This is not a valid physical description given that the microscopic dislocation mechanism for the non-recoverable kinematics of crystal material deformations creates discontinuities between atomic planes of grains in a material sample. In addition, the mathematical structure of available continuum kinematic metrics is deterministic. This is also not physically realistic because the physical numbers per unit volume per unit species volume for both the stochastic dislocation density and stochastic grain lattice structure density functions are best described as classical probability density functions in a spatial, time, and species variable domain. A stochastic descriptive for dislocation density has been developed, and explicitly introduced in a finite deformational functional (Stout, 1981). This finite deformational functional is extended to include an explicit dependence on a stochastic grain lattice structure density function. In the analyses, stochastic evolution equations are derived for both the dislocation density and the grain lattice structure density functions. Finally, the analyses of this dislocation-grain deformational functional provide stochastic kinematic metrics that contain length scale measures based on the physical attributes of both dislocations and grains. These derivations address the fundamental material response issue of representing physical deformation mechanisms by applying mathematically descriptive and consistent analyses. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48. (file-MRSdislABS102) Lee, E.H. (1970): Plastic-Wave Propagation Analysis and Finite Elastic-Plastic Theory at Finite Deformation, (page 3-29), Shock Waves and the Mechanical Properties of Solids, Ed. J.J. Burke & V. Weiss, Syracuse University Press. Stout, R.B. (1981): Modelling the deformations and thermodynamics for materials involving a dislocation kinetics, Crystal Lattice Defects, 9, pp65-91.

W5.28

COMPRESSION TESTING OF Ta SINGLE CRYSTALS. Christopher Bull, Clyde Briant, Division of Engineering, Brown University, Providence, RI; and D. Lassila, Lawrence Livermore National Labs, Livermore, CA.

This paper will report a study of deformation of tantalum single crystals in compression. Crystals oriented with 001 and 125 directions parallel to the compression axis were examined, and particular attention was given to samples that were prestrained in the 001 direction at 873K and the tested in then 125 direction. The 125 direction was chosen because it should give a maximum amount of single slip. Tests were performed over a range of strain rates (.0001 to 1 /s) and temperature (193 to 375K). Interferometric measurements were made on the sides of the crystals to examine the details of barreling. These results will be interpreted in terms of models for dislocation motion in bcc metals. The work at Brown University was supported by Lawrence Livermore National Labs.

W5.29

DISLOCATION LOOP STRUCTURE, ENERGY AND MOBILITY OF SELF-INTERSTITIAL ATOM CLUSTERS IN VANADIUM. Luis A. Zepeda-Ruiz, Brian D. Wirth, Jaime Marian, Lawrence Livermore National Laboratory, MSTD/CMS, Livermore, CA; David J. Srolovitz, Princeton Materials Institute, Princeton University, Princeton, NJ.

Isolated self-interstitial atoms (SIA) and SIA clusters that are produced in displacement cascades have significant impact on the microstructural evolution under neutron and high-energy charged particle beam irradiations. In the present study, we use molecular-statics and molecular-dynamics (MD) simulations based on a new Finnis-Sinclair potential to model the energy and mobility of SIA clusters in vanadium. The results are compared to experimental observations and recent results in Ferritic alloys which detail the formation mechanism responsible for the nucleation and growth mechanism of $< 100 >$ dislocation loops. In particular, we provide an explanation for the fact that $< 100 >$ loops are not observed in Vanadium. The SIA clusters are composed of $< 111 >$ split dumbbells and crowdions. The clusters can be described as perfect prismatic dislocation loops with Burgers vector $b = (a/2) < 111 >$. As the loops grow, SIAs fill successive jogged edge rows with minimum free energy cusps found at the magic numbers corresponding to un-jogged filled hexagonal shells. The total energy of the clusters is in excellent agreement with continuum elasticity dislocation theory predictions. The SIA clusters are highly mobile and undergo one-dimensional motion on their glide prism. The high cluster mobility is related to the easy motion of the edge segments, which propagate the kinks along the loop periphery resulting in increments of prismatic glide. Linking atomistic point defect cluster calculations, dislocation theory and experimental results provides a powerful tool in understanding radiation damage.

W5.30

A MECHANISIM-BASED CONTINUUM MODEL FOR SINGLE CRYSTAL CYCLIC PLASTICITY. Biqiang Xu, Yanyao Jiang, Department of Mechanical Engineering, University of Nevada, Reno, NV.

A mechanism-based constitutive model was developed to bridge the cyclic plasticity behavior of a single crystal and the corresponding characteristic dislocation structures. The yield and flow rules were built on the individual slip systems. The additive Armstrong-Frederick type kinematic hardening rule was adopted to capture the Bauschinger effect in cyclic plasticity. A material memory parameter was introduced to consider the amplitude dependence of cyclic hardening. Latent hardening considering the interactions among the slip systems was used to model the anisotropic cyclic plasticity behavior of a single crystal. Experimental observations on the cyclic plasticity behavior of the copper single crystals were used to evaluate the model developed. It was found that the model was able to adequately describe the well-known three distinctive regions in the cyclic stress-strain curve of a single slip oriented FCC single crystal and the associated dislocation structures for these regions. The model was capable of capturing the enhanced hardening observed in the copper single crystals in the multi-slip orientations. As a result, the anisotropic cyclic plasticity properties of a single crystal can be properly described. For a given loading history, the model was able to predict not only the saturated stress-strain responses but also the detailed evolution of the transient cyclic behavior. The characteristic dislocation structures of the copper single crystal can be reasonably featured with the state variables built into the model.

W5.31

A DISLOCATION MODEL FOR NUCLEATION DURING RECRYSTALLIZATION. Elizabeth A. Holm, Materials and Process Modeling, Sandia National Laboratories, Albuquerque, NM; Mark A. Miodownik, Department of Mechanical Engineering, King's College London, London, UNITED KINGDOM.

During or after plastic deformation, dislocations may organize into compact structures such as cell walls in a process termed recovery. If sufficient stored energy remains, the material may recrystallize by nucleating and propagating dislocation-free grains. The process by which a recovered dislocation structure gives rise to growing, strain-free grains has been debated for several decades. In this paper, we present a new model for the nucleation of recrystallized grains from a recovered subgrain structure. The model incorporates subgrain topology, boundary distribution and boundary properties to derive a nucleation frequency. The nucleation event is found to be mobility-driven discontinuous growth of certain subgrains. Microstructural predictions of the model are tested on subgrain structures in plastically deformed aluminum, using experimentally

measured subgrain characteristics. Excellent phenomenological agreement between the model and the experiments is observed. This nucleation model may also be applied to larger-scale process models of recrystallization. We present an example of a recrystallization model for aluminum nitride tube steels during hot working, which incorporates the nucleation model into a continuum mechanics framework.

W5.32
EVOLUTION OF THE DEFECT MICROSTRUCTURE IN FATIGUED Si SINGLE CRYSTALS. Marc Legros, CEMES, Toulouse, FRANCE; Olivier Ferry, Jean-Pierre Feiereisen, Alain Jacques, Amand George, LPM, Nancy, FRANCE.

The mechanical behavior of single crystals in fatigue has been investigated intensively in the fcc metals, to a lesser extent in bcc metals and very little in semiconductors. Fatigue is a deformation mode that produces specific self-organized dislocation arrangements. Combining the slip modes of fcc metals, a rather large dislocation dissociation width (comparable to Cu), and a large lattice friction (as in most bcc metals), silicon is an attractive material for new fatigue experiments. We report on tension/compression uniaxial testing of single crystalline Si, oriented for single slip conditions, between 800 and 900°C, where the lattice friction remains significant. Both the mechanical behavior and corresponding dislocation arrangements differ significantly from what was observed in metals so far. Cyclic stress-strain curves exhibit two different stages of hardening and pass through a marked maximum before saturation is reached. At variance of what is observed in metals, both the saturation stress and the cumulative strain at which this saturation occurs are lowered when the strain amplitude per cycle is increased. SEM observations suggest that strain localization takes place near the maximum stress and beyond. A structure consisting of prismatic loops has been observed exclusively in samples that reached stress saturation. This structure may be characteristic of zones that annealed after becoming inactive, and could therefore confirm the occurrence of a strain localization elsewhere in the crystal. The so-called persistent slip bands (PSB) found in fcc metals, with a condensed walls configuration, were only scarcely observed. The vein structure as described in fcc metals was not found, but a wall thickness reduction, similar to a condensation process was observed and could be responsible for the stress saturation. This remains to be confirmed since TEM observations revealed a variety of dislocation arrangements.

W5.33
MEASUREMENT OF PLASTIC DEFORMATION IN THREE-DIMENSIONS USING MICRON RESOLUTION X-RAY STRUCTURAL MICROSCOPY. B.C. Larson, Wenge Yang, G.E. Ice, J.Z. Tischler, J.D. Budai, W. Liu, Oak Ridge National Laboratory, and G.M. Pharr, University of Tennessee, Knoxville and Oak Ridge National Laboratory.

A recently developed differential-aperture x-ray structural microscopy (DAXM) technique has been used to study plastic strains and deformation microstructure distributions in nanoindented copper. The DAXM technique for submicron resolution studies of plastic deformation and the potential for direct linkage of these DAXM measurements with computer simulations and multiscale modeling on mesocopic length scales of tenths of microns to hundreds of microns will be discussed. Micron resolution 3D structural microscopy measurements of deformation microstructure in Berkovich indented Cu (made at the UNICAT beamline of the Advanced Photon Source) will be presented. These measurements will be used to illustrate the sharp differences that exist between simple models of nanoindentation and the inhomogeneous nature and the extended spatial of extent of deformation measured under nanoindents in this ductile material. This research was sponsored by the US Department of Energy, Basic Energy Sciences, Division of Materials Sciences under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, managed by UT-Battelle, LLC; The operation of the APS is sponsored by the DOE. UNICAT is supported by the Univ. of IL-MRL, Oak Ridge National Lab., National Institute for Standards and Technology, and UOP, Inc.

W5.34
3D MEASUREMENT OF DEFORMATION MICROSTRUCTURE UNDER SPHERICAL NANOINDENTS IN Cu USING X-RAY MICROBEAMS. Wenge Yang, B.C. Larson, G.M. Pharr, J.D. Budai, G.E. Ice, J.Z. Tischler, and W. Liu.

We have used white x-ray microbeams and differential-aperture x-ray microscopy (DAXM) on the UNICAT beamline of the Advanced Photon Source to perform micron-resolution three-dimensional measurements of the deformation microstructure spherical nanoindents in $< 111 >$ oriented single crystal Cu. Measurements of local orientations and geometrical necessary dislocation (GND) distributions were made with micron resolution on 35 micron deep by 50 micron long slices through the diameter of nanoindents made with a 69 micron sphere and forces ranging from 12.5 to 400 mN. Plastic deformation was found to be strong near the indent surface, but significant dislocation banding and sharp lattice rotations were found to penetrate deep into the Cu crystal. The rotations and the extent of deformation scaled with the indent force and they were found to be largely radial, dominated by the cylindrical symmetry of the indent geometry. Quantitative rotation and GND results will be presented and discussed in connection with available finite-element modeling predictions for nanoindents. This research was sponsored by the US Department of Energy, Basic Energy Sciences, Division of Materials Sciences under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, managed by UT-Battelle, LLC; The operation of the APS is sponsored by the DOE. UNICAT is supported by the Univ. of IL-MRL, Oak Ridge National Lab., National Institute for Standards and Technology, and UOP, Inc.

W5.35
Abstract Withdrawn.

W5.36
APPLICATION OF THE 3D X-RAY CRYSTAL MICROSCOPE TO STUDY MESOSCALE STRUCTURE OF MATERIALS. Gene E. Ice, Bennett C. Larson, Fred Walker, Oak Ridge National Laboratory, Oak Ridge, TN.

The 3D x-ray crystal microscope is an emerging new tool for the study of mesoscale structure in polycrystalline materials. With this nondestructive device, local crystalline orientation, phase, elastic and plastic strain tensors can be measured with submicron spatial resolution in three dimensions. A key step in analyzing the Laue patterns from the 3D microscope is indexing the reflections which determines the orientation of the sub-grain. With current algorithms, the angles between pairs and triplets of reflections are compared to theoretical angles to make guesses as to the reflection index. The ability to index a pattern can however be compromised by both elastic and plastic deformation of a grain; elastic deformation changes the angles between reflections and plastic deformation increases the uncertainty in the centroid of each reflection. Here we report on the use of an indexing algorithm that simultaneously fits all peaks. This algorithm is far more robust than previous methods and allows for robust indexing of highly deformed or strained grains. Some applications to studies of mesoscale materials properties are described.

W5.37
HIGH PRESSURE, ANHARMONIC THERMOELASTICITY OF TANTALUM. Daniel Orlikowski, Per Söderlind, and John A. Moriarty, Lawrence Livermore National Laboratory (LLNL), Livermore, CA.

The elastic moduli for bcc tantalum have been investigated over broad ranges of pressure (10 Mbar) and temperature (12,000 K), using first-principles methods that account for the cold, electron- and ion-thermal contributions. In this approach, the full potential linear muffin-tin orbital (FP-LMTO) method for the cold and electron-thermal contributions is combined with closely coupled atomistic simulations for the ion-thermal contribution, using quantum-based interatomic potentials derived from model generalized pseudopotential theory (MGPT) for the latter. While the harmonic part of the ion-thermal contribution can be readily obtained from strain derivatives of quasi-harmonic phonons, we have developed a more general Monte Carlo (MC) simulation method for the corresponding anharmonic part. The MC method directly calculates the elastic moduli through a fluctuation formula comprised of averages in the canonical distribution. Available results will be compared with ultrasonic measurements and diamond-anvil-cell compression experiments as functions of temperature and pressure. Also, the importance of these results in context to larger-scale constitutive models like the Steinberg-Guinan strength model will be discussed. 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 W-7405-Eng-48.

SESSION W6: MULTISCALE MODELING OF MICROSTRUCTURES AND EXPERIMENTS
Chairs: Lyle E. Levine and Dan Nikkel
Thursday Morning, April 24, 2003
Franciscan II/III (Argent)

8:30 AM *W6.1
TENSILE TESTS ON COLUMNAR GRAIN STRUCTURES IN TANTALUM. B. El-Dasher, Dept. of Materials Engineering, Carnegie Mellon University, Pittsburgh, PA; B.L. Adams, Dept. of Mechanical Engineering, Brigham Young University, Provo, UT; and A.D. Rollett, Dept. of Materials Engineering, Carnegie Mellon University, Pittsburgh, PA.

We report on tensile tests performed on thin sheet samples of tantalum that have a columnar structure. By annealing sheet of approximately 1 mm at high temperatures, a columnar structure is generated with grain boundaries nearly perpendicular to the flat surfaces. Automated electron back-scatter diffraction (EBSD) has been used to obtain orientation maps both before and after deformation. For the small strains used in this study (<10%), the grains deform rather uniformly with little evidence of cell formation. Analysis of the lattice rotations shows considerable scatter in the rotation axis and poor agreement with polycrystal plasticity calculations. The purpose of the experiments is to investigate the plastic response in terms of crystal plasticity in a geometry that is readily amenable to both experimental characterization and computer simulation. By linking knowledge of single slip system behavior to polycrystal response in a specific geometry, one link in the multiscale modeling of materials behavior can be validated.

9:00 AM W6.2
A POLYCRYSTAL PLASTICITY MODEL FOR F.C.C. MATERIALS WITH SUBSTRUCTURE-EVOLUTION BASED HARDENING. S. Mahesh, I.J. Beyerlein, C.N. Tomé, R.J. McCabe, A. Misra, Los Alamos National Laboratory, Los Alamos, NM.

Polycrystal plasticity models which predict macroscopic flow behavior and texture evolution in materials under various loading conditions through grain-level calculations have relied upon empirical hardening rules such as the well-known Voce law. Many works in recent years (e.g., Peeters et al. [1]) have aimed at replacing such empirical relationships with substructure-evolution based models. These models keep track of one or more families of dislocations (such as mobile cell dislocations, immobile cell block dislocations etc.) by evolving them according to well-defined laws. These laws involve several parameters which determine dislocation generation, trapping, annihilation, etc. The parameters, which form the bridge between vastly different length scales, are determined experimentally. The aim then is to capture computationally in as few parameters as possible, not only the grain's hardening behavior, but also the substructure evolution of the individual grains, as may be observed by microscopy. The modern substructure-based approach captures features of the macroscopic behavior such as the Bauschinger effect upon strain reversal, which the classical empirical methods do not. We will present a model and supporting experiments for such a study carried out on F.C.C. Copper. The model takes into account among others, grain orientation, grain-grain interactions, and strain-rate and temperature dependence. We extend the substructure evolution model of [1] for BCC Steel to FCC Cu and the associated model parameters are fit so that the predicted macroscopic data agree with experiment under different loading conditions, including strain path changes. Agreement betweeen model predictions and experiment are used as a test for the model and parameters as a general descriptor of the material. [1] Peeters et al, Acta mater, 49 (2001). 1607-1619.

9:15 AM W6.3
HOW TO GROUND MULTISCALE MATERIALS MODELS IN REALITY. David Basanta, Mark A. Miodownik, Department of Mechanical Engineering, King's College London, London, UNITED KINGDOM; Elizabeth A. Holm, Materials and Process Modeling, Sandia National Laboratories, Albuquerque, NM.

The structure-property link is an important cornerstone of mechanical modelling and is one of the main driving forces for the development of methods such as molecular dynamics, dislocation dynamics, phase field methods, and finite element simulations. In all these methods, the spatial and temporal modelling of microstructure is the key to predicting properties. The sensitivity of the properties to the configuration of the initial microstructure is not often studied. Performing such a sensitivity analysis is important when making the leap from model development to model application. It is also vital that the initial microstructures come from microscopy of the applied system. In two dimensions (2D) this is relatively straightforward, since microstructures can be imaged in 2D at various length scales by a number of well-known techniques, including scanning electron microscopy (SEM), transmission electron microscopy (TEM) and atomic force microscopy (AFM). But in three dimensions (3D) it is problematic because getting 3D information is experimentally very challenging. Oddly it is only at the atomic scale that 3D experimental techniques are sufficiently developed, e.g. atom probe techniques. In this paper we will discuss a general approach to solving this problem of generating initial structures for simulations. We will describe a program called MicroConstructor, which will take 2D micrographs and generate statistically equivalent 3D computer microstructures. The basis of the code is a genetic algorithm that evolves the 3D microstructure so that its cross-sections match the 2D data. Since this approach is not limited by scale, it will enable multiscale microstructural modellers to use as their starting point realistic 3D microstructures without having to acquire 3D information experimentally, a very time consuming and expensive process.

9:30 AM W6.4
EFFECTS OF GRAIN BOUNDARY CONSTRAINT ON THE CONSTITUTIVE RESPONSE OF TANTALUM BICRYSTALS. Alexander Ziegler, Geoffrey H. Campbell, Mukul Kumar, Material Science and Technology Division, Lawrence Livermore National Laboratory, Livermore, CA; James S. Stölken, New Technologies Engineering Division, Lawrence Livermore National Laboratory, Livermore, CA.

The role of grain boundary constraint in strain localization, slip system activation, slip transmission, and the concomitant constitutive response was examined performing a series of uniaxial compression tests on tantalum bicrystals. Tantalum single crystals were diffusion bonded to form a (110) twist boundary and compressed along the [110] direction. The resulting three-dimensional deformation was analyzed using a combination of volume reconstruction and surface grid evaluation. Both, the effective states of stress and strain over the cross-sectional area could be measured as a function of distance from the twist boundary. Local strains and strain gradients were measured as a function of position on the surface of the test specimen. Post-test metallurgical characterization was performed using Electron Back-Scattered-Diffraction (EBSD). The results, a spatial distribution of slip patterning and mapping of crystal rotation near the twist-boundary was analyzed and compared to the known behavior of the individual single crystals. The detailed shape change and lattice rotation measurements were compared with finite element simulations. The influence of the constraint induced multiaxial stress-state on the constitutive assumptions of crystal plasticity shall be critically examined.

9:45 AM W6.5
A STATISTICAL CONNECTION BETWEEN DISLOCATIONS AND MECHANICAL PROPERTIES. L.E. Levine and Robb Thomson (retired), Metallurgy Division, National Institute of Standards and Technology, Gaithersburg, MD.

The changes in mechanical properties that occur during the plastic deformation of metals result from the complex interaction of huge numbers of mobile and immobile (trapped) dislocations. The dislocations interact via long-range, 1/r, angle-dependent stress fields that become highly non-linear at short range. In spite of this underlying complexity, mechanical property measurements exhibit a relatively simple and consistent behavior, requiring only a few internal state variables for reasonably accurate simulation. This drastic simplification arises because a deforming metal can be described as a self-organizing critical system where the correct internal state variables are actually statistical parameters dealing with how mobile dislocations are produced and how they interact with cell walls. This process is controlled by the continuously evolving distribution of dislocation segment lengths, allowing us to connect the system behavior to time, temperature, applied stress, strain, and strain rate.

10:30 AM W6.6
MICRODIFFRACTION EXPERIMENTS AND MODELING FOR ANALYZING MULTISCALE DISLOCATION ENSEMBLES IN MATERIALS. Gene Ice, Rosa Barabash, Oak Ridge National Laboratory, Metals and Ceramics Div, Oak Ridge, TN.

Ultra-brilliant 3rd generation synchrotron sources can be used to probe local crystalline structure with submicron spatial resolution. White-beam X-ray microdiffraction using Kirkpatrick-Baez focusing optics and an x-ray sensitive CCD area detector was applied to understand the dislocation structure arising from plastic deformation. We show how unpaired dislocations alter the white beam Laue patterns for either isolated dislocations, dislocation walls, or combinations of dislocation walls and isolated dislocations. The intensity distribution of Laue diffraction is analyzed as a function of local misorientation. The influence on the Laue pattern for the 12 most likely FCC slip systems can be distinguished because of their distinctly different streaking directions. The condition that leads to splitting of Laue spots is discussed. As resolution increases, experimental sensitivity to the hierarchical arrangement of dislocations also increases. We describe various strategies to quantitatively determine the best-fit parameters for dislocation density, slip system, fragment positions and misorientation angles through GNBs between scattering fragments. With the fitted parameters, we can simulate the whole Laue pattern including details about the contours for specific Laue spots; good agreement is found between simulated and experimental contours. Uncertainties with the current approach and future improvements are discussed.

10:45 AM W6.7
ACCOMMODATION OF COHERENCY STRAIN BY INTERFACIAL DISCONNECTIONS AT A 90 DEGREE GRAIN BOUNDARY IN GOLD. D.L. Medlin and D. Cohen, Sandia National Laboratories, Livermore, CA; R.C. Pond, Dept of Engineering (Materials), University of Liverpool, Liverpool, UNITED KINGDOM.

The specific mode by which strain is accommodated at a grain boundary depends ultimately on the defects that are admissible at the interface. Therefore, understanding the structure and topology of such defects is vital to connecting atomistic and mesoscale descriptions of grain boundary behavior. In this presentation we discuss the structure of interfacial disconnections (i.e. line defects possessing both step and dislocation character) at a 90 degree < 110 > tilt boundary in gold. This grain misorientation is interesting because while it aligns several pairs of low index planes and directions, the ratios of periodic lengths in all the parallel directions (with the exception of the shared < 110 > axis) are irrational. High resolution transmission electron microscopy (HRTEM) observations identify these defects separating short (4-6 nm) (111)/(112) terraces along the boundary. By measuring the dislocation content of the disconnections, we show how the defects accommodate the 5.7% "misfit" in the directions parallel to the interface and thereby enable coherency across the (111)/(112) terraces. This structural relaxation is markedly different from that at (100)/(110) grain boundary facets in this same system, for which previous observations have found an incoherent structure with no strain localization. The comparison between these two cases points to the very important coupling between grain boundary inclination and the particular mode by which incompatibilities between adjacent grains are accommodated. Furthermore, this work illustrates the importance of specifying the reference state in characterizing the topological properties of a disconnection, a result that is of general importance to modeling interfacial defects.

11:00 AM W6.8
CAPTURING THE INFLUENCE OF GRAIN BOUNDARIES IN POLYCRYSTAL PLASTICITY MODELING. Thomas E. Buchheit, Gerald W. Wellman, Corbett C. Bataille, Sandia National Laboratories, Albuquerque, NM.

A material model which uses a crystal plasticity framework has been implemented into a quasistatic finite element code to realize microstructure-based polycrystal plasticity simulations. The resultant finite element model has successfully performed 3-D simulations of realistic polycrystalline microstructures containing hundreds of grains and as many as 100,000 elements. However, the simulations lack a length scale creating a variety of issues including their inability to capture the influence of grain size, an element-size to grain-size mesh dependence and a limited phenomenology that is incapable of accurately predicting the evolution of deformation substructure within grains. To address these issues, a model has been devised and implemented into the original material model framework that contains a gradient in strength near grain boundaries. This new model provides a length scale within the polycrystalline material response that captures the influence of grain size and eliminates mesh dependence. In addition, various forms of this model can be implemented that capture Hall-Petch breakdown and the mechanical response of nanocrystalline materials in polycrystalline simulations. Finally, the deformation substructure evolves in a manner that more closely resembles experimental observations. The presentation will conclude with results from this first example of predicted deformation substructure evolved using a polycrystal plasticity model. *Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-ACO4-94AL85000.*

11:15 AM W6.9
MODELING RADIATION DAMAGE EFFECTS ON THE DUCTILITY OF POLYCRYSTALLINE METALS.
Athanasios Arsenlis, Moono Rhee, Meijie Tang, Lawrence Livemore National Laboratory, Livermore, CA; Brian D. Wirth, University of California Berkeley, Berkeley, CA.

Nuclear reactor environments induce the development of nanometer scale defects that affect the mechanical behavior at macroscopic length scales. To develop an internal state variable-based isotropic plasticity model for materials subject to these environments an information passing multi-scale modeling materials framework is adopted in which the final coarse-grained model is informed by finer simulations at smaller length scales. Experimental observations have shown that the irradiation induced defect structures depend on irradiation fluence, fluence rate, temperature, and dosage. The defects observed are composed of clusters of vacancies that may organize to from stacking fault tetrahedra and/or prismatic dislocation loops. Molecular dynamics simulations of the interaction between a stacking fault tetrahedron (SFT) and an isolated dislocation are conducted to investigate the effect of a density SFTs on the motion of dislocations and the evolution of SFT's during dislocation glide. Dislocation dynamics simulations are conducted in the absence of irradiation induced defect structures to investigate dislocation density multiplication and growth mechanisms that operate at the onset of plastic deformation in single crystals. The mechanisms for dislocation density growth and multiplication and for irradiation damage defect evolution and dislocation interaction are incorporated into a dislocation density-based isotropic plasticity model. The final coarse-grained model is implemented into a finite element framework and used to simulate the behavior of tensile specimens with varying levels of irradiation induced material damage. Comparison of simulation results with experimentally observed mechanical behavior of irradiated materials compares favorably in terms of predicting increased strength, decreased hardening, and decreased ductility within increasing irradiation dosage. 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.

11:30 AM W6.10
ON THE SINK STRENGTH FOR POINT DEFECTS OF NANOSIZED GRAIN BOUNDARIES. M. Samaras, P.M. Derlet, H. Van Swygenhoven, Paul Scherrer Institut, Villigen-PSI, SWITZERLAND; M. Victoria, Fusion Technology-CRPP-EPFL, Villigen-PSI, SWITZERLAND.

It is well known that grain boundaries (GB) act as sinks for intersitial atoms created during irradiation and that this results in a denuded zone around the GB. Experiments and modelling confirm this trend, showing a defect-free zone of about 3 to 20nm around a discrete dislocation. Molecular dynamics simulations are performed to study defect production in irradiated nanocrystalline Ni with mean grain sizes of 5, 12 and 20nm. It is shown that the interstitials are attracted to GBs by means of replacement collision sequences to these areas where misfit is accommodated by GB dislocations and excess free volume is present. Moreover, stacking fault tetrahedra are easily formed in the nanosized grains, which would result in material hardening. The sink strength of GBs is investigated in terms of grain size and the non-equilibrium state of the GBs. (PRL 88 (2002)125505, Phil. Mag. A (2002) in press).

11:45 AM W6.11
MESOSTRUCTURE OF TEXTURED METAL MATERIALS: EXPERIMENTAL STUDY AND NEW-DISCOVERED REGULARITIES. Yuriy Perlovich, Margarita Isaenkova, Vladimir Fesenko, Moscow Engineering Physics Institute, Dept of Physical Problems of Materials Science, Moscow, RUSSIA.

Different structural levels in metal materials are controlled by independent regularities, which can be revealed only by use of proper experimental methods. The main feature of the mesolevel is a sharp substructure inhomogeneity, observable by the comparison of grains with different orientations. In order to study systematically the substructure inhomogeneity of textured materials, an X-ray method of Generalized Pole Figures (GPF) was developed. The method consists in registration of the X-ray line profile by each successive position of the sample in the course of texture measurement, so that for grains of all orientations diffraction or substructure parameters are measured. Since the physical half-width of X-ray line depends on fragmentation of grains / distortion of their crystalline lattice and the peak position is determined by interplanar spacing along the normal to reflecting planes, GPFs of half-width and peak position give the fullest accessible description of substructure, formed in metal materials with deformation textures. Analysis of obtained distributions as applied to many rolled metal materials resulted in the following general conclusions: (1) The structure of deformed metal includes an extremely wide spectrum of substructure conditions. (2) The crystallographic orientation of grains is the most effective criterion for systematization of substructure inhomogeneities in textured materials. (3) Grain fragmentation and lattice distortion are minimal in texture maxima and increase up to highest values by passing to texture minima. (4) The distribution of lattice elastic deformation shows in the orientational space a cross-wise pattern, that is alternation of quadrants with predominance of elastic extension or elastic compression, providing an equilibrium of microstresses relative to the symmetry planes of the rolling scheme. Substructure differences between texture maxima and texture minima are explained on the basis of texture formation models by introducing the concepts of orientation stability, successive retardation and activation of slip systems, fragmentation of grains due to fluctuations of their orientation about the stable position.

SESSION W7/U8: JOINT SESSION
MODELS AND EXPERIMENTS IN NANOSTRUCTURED MATERIALS
Chairs: Helena Van Swygenhoven and Hussein M. Zbib
Thursday Afternoon, April 24, 2003
Metropolitan I (Argent)

1:30 PM W7.1/U8.1
MULTISCALE MODELING OF VOID GROWTH IN DUCTILE

METALS. Robert E. Rudd, Eira T. Seppälä, James Belak, Lawrence Livermore National Laboratory, Livermore, CA; Marc C. Fivel, CNRS/INPG, Domaine Universitaire, Grenoble, FRANCE.

Void growth is an important microscopic process in the fracture of ductile metals. Several well-established models are commonly used to describe the development and evolution of void populations through a coarse-grained porosity, but detailed models of void growth with atomic-level specificity have not been available. As the first steps in a hierarchical approach to the modeling of void growth associated with dynamic fracture, we have developed atomistic and mesoscale models [1,2] that describe the evolution of voids under an applied tension. In our simulations this tension arises from expansion at a constant strain rate for comparison with dynamic fracture experiments conducted at LLNL and elsewhere. The hierarchical approach in effect replaces the empirical constitutive relations used in continuum modeling of void growth with classical interatomic force laws, and the elastic and plastic behavior of the metal is derived from the collective response of the atoms. In this talk we compare the evolution of the plastic zone surrounding a growing void for several different ductile metals, including both face-centered-cubic (FCC) and body-centered-cubic (BCC) transition metals. In particular we analyze the character of the dislocation activity, and we contrast the details of this plastic response for several metals. The dislocation characterization and nucleation rules are used to inform a dislocation dynamics simulation in order to extend to longer length scales and slower strain rates. Acknowledgment: This work was performed under the auspices of the US Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48. [1] J. Belak, "On the nucleation and growth of voids at high strain-rates," J. Comp.-Aided Mater. Design 5, 193 (1998). [2] R.E. Rudd and J. Belak, "Void Nucleation and Associated Plasticity in Dynamic Fracture of Polycrystalline Copper: An atomistic simulation," Comput. Mater. Sci. **24**, 148 (2002).

1:45 PM W7.2/U8.2
GRAIN BOUNDARY PROCESSES DURING DEFORMATION OF NANO-SCALE GRAIN BOUNDARY MICROSTRUCTURES: ATOMISTIC SIMULATION STUDIES. Moneesh Upmanyu, Material Science Program, Division of Engineering, Colorado School of Mines, Golden, CO; and B. Radhakrishnan, Computational Materials Science Group, Oak Ridge National Laboratory, Oak Ridge, TN.

We have performed molecular dynamics simulations of deformation of bicrystals in pure Al to study the mechanism of strain accommodation at nano-scale grain boundaries. We first investigate dislocation nucleation as a function of the strain imposed on the bi-crystal. Detailed analyses of the grain boundary structure before and after deformation (in the elastic as well as plastic regimes) are carried out to arrive at the atomistic mechanisms of strain accommodation. The spatio-temporal variation of excess grain boundary quantities such as grain boundary enthalpy, volume, etc., are investigated to determine the dependence of the strain accommodation mechanisms on bi-crystallography. Finally, the effects of such strain accommodation mechanisms on nano-scale plasticity are discussed.

2:00 PM W7.3/U8.3
MOLECULAR DYNAMICS SIMULATIONS OF VOID GROWTH IN DYNAMIC FRACTURE OF FCC AND BCC METALS.
Eira T. Seppälä, James Belak, Robert E. Rudd, Lawrence Livermore National Laboratory, Livermore, CA.

Dynamic fracture in ductile metals occurs commonly through the nucleation and growth of voids, with concomitant dislocation formation and propagation. Here we have studied at the atomistic scale the growth of a pre-existing spherical void initially a few nanometers in radius in single-crystal face-centered-cubic (FCC) and body-centered-cubic (BCC) lattices under dilational strain. Molecular dynamics (MD) simulations using an Embedded-Atom-Model (EAM) potential to model copper and a Finnis-Sinclair potential to model tantalum have been performed at high strain-rates ranging from 10^6/sec to 10^{10}/sec. We have especially concentrated on the quantitative analysis of the void shape evolution depending on the stress-triaxiality by varying the loading as uniaxial, biaxial, and triaxial expansion. The strain-rate dependence, differences between lattice structures, and the structures of dislocations, which emerge from the void and lead to its growth, have been investigated, too. These atomistic-level studies, which are done at initial system sizes about $[25\ \mathrm{nm}]^3$ and starting from room temperature, have been compared with continuum calculations and measures such as plastic strain. Also simulations of much larger length-scales, e.g. utilizing a parallel MD code, in order to study several voids are discussed. Acknowledgment: This work was performed under the auspices of the US Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

2:15 PM W7.4/U8.4
MEASUREMENTS OF SIZE SCALE EFFECTS IN LAYERED STRUCTURES. Ashraf Bastawros, Antonia Antoniou, Iowa State Univ, Dept of Aerospace Engineering and Engineering Mechanics, Ames, IA.

A novel experimental configuration is devised to measure the evolution of the deformation field and the corresponding toughness evolution within soft metallic films constrained by hard layers. The experimental configuration provides pure shear state within the constrained film. The material system utilized comprised ductile layer of Tin based solder, encapsulated within relatively hard copper shoulders. Different Tin-Lead compositions are tested with grain size approaching the film thickness. The in-plan strain distribution within the film layer is measured by a microscopic digital image correlation system. The toughness evolution within such highly gradient deformation field is monitored qualitatively through a 2D surface scan with a nano-indentor. The measurements showed a highly inhomogeneous deformation field within the film with discreet shear bands of concentrated strain. The localized shear bands showed long-range correlations of the order of 3-4 the grain size. A size-dependent macroscopic response on the layer thickness is observed. However, the corresponding film thickness is approximately 100-1000 times larger than those predicted by non-local continuum theories and discreet dislocation.

2:30 PM W7.5/U8.5
TWO BRANCH UNIVERSAL BINDING ENERGY RELATIONSHIP FOR RELAXED SURFACES. Robin L. Hayes, Emily A.A. Jarvis, Emily A. Carter, University of California, Los Angeles, Department of Chemistry and Biochemistry, Los Angeles, CA.

In 1983, Rose, Smith and Ferrante proposed a Universal Binding Energy Relationship (UBER) to describe the bonding between unrelaxed surfaces of many materials. Since then, UBER has been extensively used to represent cohesion between crack surfaces in continuum models. Unfortunately, the traditional UBER model is incapable of capturing the substantial reduction in surface energies often caused by surface relaxation. We ran a series of Density Functional Theory (DFT) calculations where we introduced a crack into a 3D periodic slab and allowed all the ions to relax. The energies of relaxed surfaces can be separated into two regimes: elastic and cracked. In the elastic regime, the introduced crack heals to form a uniformly expanded solid characterized by a chain of harmonic springs if the two surfaces are close enough for the electron density to bridge the gap. In the cracked regime, the traditional UBER functional form captures the correct behavior if the actual interplanar separation between *relaxed* surfaces is used and the energy is shifted to match the relaxed surface energy. Al and Al_2O_3 display extremely different mechanical behavior which provides a stringent test of the universality of our model. Specifically, (0001) α-Al_2O_3 is a brittle ceramic whose surface ions relax inward by nearly 1 $\AA$, while (111) fcc Al is a ductile metal whose surface ions relax slightly outward by 0.1 $\AA$. Both materials are well described by our 2-branch model. A Taylor expansion of the traditional UBER reveals that both harmonic and anharmonic terms are needed to fit DFT energies that should be purely harmonic. This leads to an artificially high elastic constant which produces errors if the traditional UBER is extrapolated to larger systems. Hysteresis arises from the nearly constant interplanar separation required for crack healing compared to the system size-dependent elastic behavior encountered prior to crack formation.

3:15 PM *W7.6/U8.6
APPLICATION OF A MODIFIED JOGGED-SCREW MODEL FOR CREEP OF TITANIUM ALLOYS AND TITANIUM ALUMINIDES.
Subramanian Karthikeyan, Gopal B. Viswanathan and Michael J. Mills, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH.

Stress exponents for creep in the range of five are typically associated with dislocation creep processes, and a strong tendency for subgrain formation. This presentation will demonstrate that there are several important alloy systems that have similar stress dependence, and yet lack this tendency for subgrain formation. Specifically, dislocations in the intermetallic compound γ-TiAl and the hexagonal close packed α-phase of the commercial Ti alloy Ti-6242 tend to be homogeneously distributed with a tendency for alignment along screw orientation. In both alloy systems, the screw dislocations exhibit a large density of pinning points, which detailed transmission electron microscopy investigation indicate are locations of tall jogs. These observations suggest that the jogged-screw model for creep should be appropriate after suitable modification for the presence of these tall jogs. A modified jogged-screw model has recently been developed as an alternative explanation for creep in these systems. The model parameters are all measurable from TEM experiments, and the model is shown to provide favorable prediction of the observed creep response for both γ-TiAl. This model has also been extended to treat

the case of the lamellar microstructures that are common in both γ-TiAl and Ti-6242 alloy systems. A physical explantion for the formation of tall jogs is also described and the potential application of this modified model to other alloy systems is discussed.

3:45 PM W7.7/U8.7
NON-STICK AND SCRATCH RESISTANCE SOL-GEL COATING FOR ALUMINUM. Linda Y.L. Wu and S.K. Chang, Singapore Institute of Manufacturing Technology, SINGAPORE.

PTFE coating has been used for aluminum molds for molding of polystyrene packaging materials. However, this coating does not meet the users' requirements on scratch resistance and durability. Sol-gel technology allows the formation of a ceramic-like material at a lower temperature, which provides higher hardness and better scratch resistance for improved durability. This paper describes a study on the syntheses of a PTFE/SOL-GEL composite material. This coating material combines the desirable non-stick and low friction properties of PTFE filler with the high scratch resistance and durability of a silica-based, ceramic-filled sol-gel material. The influences of colloidal silica, PTFE, aluminum oxide and titanium oxide fillers on the coating's non-stick, friction and scratch properties are investigated. This sol-gel coating is applied to grit-blasted aluminum plates by spraying. The type of solvent used in the coating solution plays an important role in non-stick and friction properties, as well as in layer build-up and crack formation. We have found the optimum combination of fillers and solvent, which gives the maximum crack-free coating thickness. From which, a greatly improved scratch-resistant coating with non-stick and low-friction properties equal to those of PTFE coatings was obtained. The scratch resistance is twice that of the PTFE coating. To further improve the scratch resistance, the grit blasting process was replaced by an electro-chemical surface treatment. This treatment leaves a porous aluminum oxide layer, which allows the sol-gel material to penetrate into its regular micro-pores (130nm), resulting in strong mechanical interlocking. The adhesion between coating and substrate has been improved significantly relative to the normal grit blasting treatment. With this adhesion enhancement, the chipping problem of sol-gel coating was solved and the scratch resistance was increased by 4 times. FE-SEM/EDX, contact angle tester, scratch tester and a pin-on-disc tribometer are used in the evaluation of the coatings properties.

4:00 PM W7.8/U8.8
STRUCTURAL EVOLUTION AND ACOUSTIC PHONON BEHAVIOR IN CRYSTALLINE PtFe LATEX FILMS. Matteo Pierno, Carlo S. Casari, Andrea Li Bassi, Marco G. Beghi, Roberto Piazza, Carlo E. Bottani, INFM - Dipartimento di Ingegneria Nucleare, Politecnico di Milano, ITALY.

The surface and bulk structural evolution of polytetrafluoroethylene crystalline polymer latex films has been studied at a length scale of few hundreds nanometers by atomic force microscopy (AFM) and Brillouin light scattering. Controlling the sintering process we observed a transition from the original particle distribution towards a 'fibrillar' structure characterized by extended crystalline regions embedded in a disordered matrix, which still retains features of the original particulate structure. This transition has led to an observed cross-over from localized acoustic excitations to propagating acoustic phonons related with the mesoscopic elastic properties. The comparison with numerical simulations of the Brillouin scattering cross section shows that fully sintered films do not yet exhibit the dynamical properties of the equivalent compact elastic continuum. This is an evidence of the persisting 'mark' of the original particulate structure after sintering, suggesting that film formation for crystalline polymers may be analogous to sintering of ceramic powders. Brillouin spectroscopy of the latter systems is often difficult due to signal weakness. The formation of films of crystalline polymers can therefore be exploited as a model system to study the elasto-optical properties of granular and disordered media. New phenomenology is thus accessible, which is also relevant for the understanding of the sintering process of ceramic powders.

4:15 PM W7.9/U8.9
GENERALIZED QUASICONTINUA: AN APPROACH TO ATOMISTIC-CONTINUUM MODELING OF COMPLEX OXIDES. Anter El-Azab, Harold Trease, James Rustad, Fundamental Science Directorate, Pacific Northwest National Laboratory, Richland, WA.

A formalism of the quasicontinuum method suitable for atomistic-continuum modeling and nanoscale mechanics of oxide crystals with basis is presented. Multiple, interacting quasicontinua, one per sublattice, which overlap in the physical crystal space are used to model complex oxide crystals. The Cauchy-Born hypothesis, which connects atomic coordinates in distorted crystals to the imposed deformation gradient, is assumed to be valid for the individual quasicontinua. Based on a Delaunay triangulation of the crystal and associated interpolation functions, the Cauchy-Born hypothesis is used to derive self-consistent coarse graining of the atomic forces of individual sublattices. Computation of forces and energy, however, takes into account the interaction among atoms on all sublattices. The method thus can be viewed as a numerical implementation of the theory of inner elasticity of crystals with basis. In this presentation, we show predictions of the structure of hematite (Fe_2O_3) crystal with and without imposed crystal distortions and compare with lattice statics method. A shell-type interatomic potential is used which accounts for the polarization of oxygen ions. In this case, the atomic shells associated with every oxygen sublattice are treated as separate sublattices, which amounts to doubling of the oxygen quasicontinua. Applications of the generalized quasicontinuum method developed here to study problems of structure and nanoscale mechanics are also discussed.

4:30 PM W7.10/U8.10
AEROSOL DEPOSITION METHOD (ADM) FOR NANO-CRYSTAL CERAMICS COATING WITHOUT FIRING. Jun Akedo, Maxm Lebedev, Astushi Iwata, Hisato Ogiso, Shizuka Nakano, Inst. of Mechanical Systems Engineering, National Inst. of Advanced Industrial Science and Technology, Tsukuba, JAPAN.

A novel method of ceramics coating based on a particle collision, named as aerosol deposition method (ADM), will be reported. Sub-micron ceramics particles were accelerated by gas flow in the nozzle up to velocity of several hundred m/s and ejected onto the substrate. During impaction and interaction with substrate, these particles formed thick (over 1μm), dense, hard and transparent ceramics layers with high deposition ratio (2 - 30 μm/min). Depositions were fulfilled at room temperature. No additional procedure for solidifications is required. The results of fabrications, microstructure and mechanical properties of oxide (Al_2O_3, YSZ, PZT etc), non-oxide materials and some composites will be presented. Hardness of PZT layer was 450 - 500 Hv, which is over that of bulk material. Hardness of Al_2O_3 layer formed at room temperature reaches 2000 Hv, which was measured by nano-indenter system and is comparable with that of bulk material. The adhesion force between the layer and the substrate was over 30 MPa. The microstructures were investigated by XRD and TEM. Every layer has polycrystalline structure with nano-meter order scale. Crystal systems of layers were same as those of starting powders. Reduction of crystallite size from sub-micron order (100 - 500 nm) to nanometer order (5 - 20 nm) was observed during collision of particles.

4:45 PM W7.11/U8.11
SYNTHESIS OF POLYMER/MESOPOROUS SILICA NANOCOMPOSITES WITH ENHANCED MECHANICAL PROPERTIES. Xiangling Ji, Eric Hampsey, Qingyuan Hu, Donghai Wang, Byron McCaughey, Xuan Li, Yunfeng Lu, Department of Chemical Engineering, Tulane University, New Orleans, LA; Weilie Zhou, Advanced Materials Research Institute, University of New Orleans, New Orleans, LA.

Organic/inorganic nanocomposites often show unique properties due to the synergies of both components. Here are report the synthesis and enhanced mechanical properties of poly((3-trimethoxysilyl)propyl methacrylate)-mesoporous silica nanocomposites. The synthesis approach involves infiltration and subsequent polymerization of the monomer (3-trimethoxysilyl)propyl methacrylate within mesoporous silica particles that are prepared using an aerosol-assisted surfactant-assembly process. Compared with poly((3-trimethoxysilyl)propyl methacrylate polymer, as synthesized nanocomposites show a small decrease in tensile strain but significantly improved tensile strength, modulus, toughness, and thermal stability. Results from scanning electron microscopy (SEM) and other characterizations suggest that entanglement of the molecular chains formed within the mesoporous channels with those in the bulk polymer may attribute to the improved mechanical properties. Since conventional polymer/inorganic composites prepared using dense silica particles as fillers often result in an improved modulus but decreased toughness, this new approach provides a unique route to fabricate nanocomposites with both reinforcement and toughening.