SYMPOSIUM A

Multiscale Phenomena in Materials–Experiments and Modeling

November 30 – December 2, 1999

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Symposium Support
Lawrence Livermore National Laboratory

**Proceedings published as Volume 578
of the Materials Research Society
Symposium Proceedings Series.**

* Invited paper

SESSION A1: PLASTICITY AT SMALL LENGTH SCALES AND CONTINUUM
Chairs: Benoit Devincre and Alan Needleman
Tuesday Morning, November 30, 1999
Room 208 (H)

8:15 AM *A1.1
PLASTICITY OF CRYSTALLINE MATERIALS AT SMALL LENGTH SCALES. W.D. Nix, Dept of Materials Science and Engineering, Stanford University, Stanford, CA.

Plastic deformation in small volumes requires higher stresses than are needed for plastic flow of bulk materials. Smaller is stronger! Predicting this well-known effect is a challenge for multiscale modeling because it involves phenomena ranging from atomics, through defect behavior to the continuum. Deformation experiments spanning these length scales are expected to provide particularly good tests for the multiscale modeling efforts currently underway. Various plasticity experiments at small length scales will be described. We show that three different, but related, effects are responsible for the high strengths of materials in small dimensions: Discrete Dislocation Effects, Fine Microstructure Effects and Strain Gradient Effects. Nanoindentation of Au single crystals at the nanometer depth scale reveals irregular load-displacement curves that appear to be associated with the nucleation of dislocations. The contact pressures at which the first inelastic events are triggered compare favorably with recent calculations of nanometer scale indentations in perfect Au crystals. We discuss special precautions that must be taken to analyze indentation experiments at this length scale. The very high strengths of thin films on substrates, compared to bulk materials, can be understood in terms of both the fine grain sizes present in these materials and the dislocation interaction processes that occur when dislocations are required to move in thin crystalline layers. Recent substrate experiments on yielding and strain hardening of thin metal films on substrates are interpreted in terms of these fine structure effects. We show that the indentation size effect for soft metal crystals can be accurately modeled using the concept of geometrically necessary dislocations . The model leads to a characteristic form for the depth dependence of the hardness, which may be interpreted as a law for strain gradient plasticity. Such a strain gradient plasticity law represents an attempt to create a continuum mechanics description of effects that are microstructural in origin.

8:45 AM *A1.2
SYMMETRY INVESTIGATION OF TEXTURED TANTALUM POLYCRYSTAL PROPERTIES. P.J. Maudlin, J.F. Bingert, Los Alamos National Laboratory, Los Alamos, NM; R.K. Garrett, Jr., Naval Surface Warfare Center, Indian Head Division, Indian Head, MD.

Several tantalum bar and plate stock materials that demonstrate mild-to-strong anisotropic plastic behavior during large deformation are analyzed in terms of tensorial property symmetry. Texture interrogations of these materials reveal duplex orientation distributions that have implications with regard to the symmetry realized in bulk plastic deformation; specifically these materials show less symmetry than one would expect from knowledge of the processing history. Mesoscale polycrystal simulations are performed to probe a general shape for the yield surfaces based on a discrete ODF representation of the material texture and previously established single-crystal deformation modes. This yield surface shape is mathematically represented in terms of second and higher-order tensors. A plastic compliance analysis is then performed to graphically map the deformation symmetry contained in these tensors for a specific choice of stress state, and the results are shown to be fully consistent with calculated anvil footprints from Taylor cylinder impact testing. Experimental texture measurements and Taylor impact results are included for validation of the overall investigative methodology.

9:15 AM A1.3
A STRAIN TENSOR AND OTHER KINEMATIC QUANTITIES AT THE ATOMIC SCALE. M.F. Horstemeyer, Sandia National Laboratories Livermore, CA; M.I. Baskes, Los Alamos National Laboratory Los Alamos, NM.

Kinematic variables used for crystal plasticity and macroscale internal state variable plasticity theories are defined and quantified in molecular dynamics Embedded Atom Method simulations. The formalism for determining the deformation gradient, velocity gradient, Green strain tensor, and plastic spin will be shown. Simulations of single crystal nickel under simple shear and tension were performed to discuss the various aspects of the kinematic quantities. Ties to crystal plasticity and macroscale internal state variable theory will be discussed as well.
This work was supported Sandia National Laboratories by the U. S. DOE under contract no. DE-AC04-94AL85000.

10:00 AM *A1.4
LATTICE INCOMPATIBILITY AND NONLOCAL CRYSTAL PLASTICITY. John L. Bassani, Dept of Mechanical Engineering and Applied Mechanics, Univ. of Pennsylvania, Philadelphia, PA.

In a wide range of plastic phenomena the overall response depends on the macroscopic size of the sample (in a non-self-similar manner) and often involves patterned (localized) flow at the microscale. At both levels the response is influenced by the magnitude of (spatial) gradients of strain relative to the total strain. For single crystals such behavior can be associated with the presence of geometrically-necessary dislocations arising from gradients in lattice deformation. In the continuum theory of crystal plasticity the lattice is assumed to distort only elastically during elastic-plastic flow, but in general this elastic deformation is not compatible with a (continuous and single-valued) displacement field. Incompatible lattice deformation requires the presence of geometrically-necessary dislocation and is characterized by a certain gradient of the elastic deformation gradient field. The latter measure can play a natural role in a nonlocal theory of crystal plasticity. A simple constitutive model where the incompatibility measure only enters the instantaneous hardening relations leads to predictions for size-scale effects in the torsion of thin wires, straining of thin films, and overall hardening of particulate composites that are in accord with observations. A comparison between this model and a discrete dislocation simulation is presented.

10:30 AM A1.5
EXPERIMENTAL STUDY OF DISLOCATION VELOCITY AND MOBILE DENSITIES. Joel Bonneville, B. Lo Piccolo-Matterstock, J.L. Martin, Ecole Polytechnique Federale de Lausanne, Department de Physique, Laboratoire de Physique Metallurgique, Lausanne, SWITZERLAND.

Plastic deformation of crystalline materials is usually described in terms of the Orowan's equation, which involves two important physical quantities: the velocity and the density of mobile dislocations. Developing a fundamental understanding of the deformation mechanisms will therefore be dependent on our ability to experimentally characterise and to model these two relevant quantities.
Conventional mechanical tests measure or impose the strain-rate, but do not allow for a separate determination of the dislocation mobility and the mobile dislocation density. Therefore, we have developed two experimental techniques based on transient tests that consist, respectively, of repeated load relaxations and, recently, of repeated creep experiments performed during constant strain-rate tests. A critical analysis of the corresponding kinetics will be given in order to properly identify the physical sense of the obtained experimental values. The significant measured parameters are the activation volume for the dislocation mobility and the mobile dislocation density resulting from the balance between dislocation multiplication and exhaustion. In addition, when exhaustion occurs with dislocation storage in the crystal, this too contributes to strain-hardening. This aspect will also be considered. Recent determination of dislocation exhaustion rates in two intermetallic compounds such as Ni_3Al of the $L1_2$ structure and TiAl of the $L1_0$ structure will be presented and critically examined. They will be compared with those of Cu. It will be shown that the relatively low work-hardening coefficient in Cu correlates well with a low mobile dislocation exhaustion rate. In contrast, this exhaustion rate is found to be high in the intermetallics and account for the large values of work-hardening. It is our hope that, in the near future, further developments of these techniques will lead to a complete characterisation of multiplication and exhaustion mechanisms occurring in the course of plastic deformation.

10:45 AM A1.6
CRYSTAL PLASTICITY ANALYSES BY ORIENTATION IMAGE MICROSCOPY AND LOCAL DEFORMATION MEASUREMENTS. Arnold Tatschl, Otmar Kolednik, Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, AUSTRIA.

We investigate in this study the evolution of the lattice orientation and the local strain fields during plastic deformation. The material is an oxygen free, high conductivity copper (OFHC). In-situ tensile tests are performed in the scanning electron microscope (SEM) where the specimens are deformed to predetermined global strain levels. Prior to deformation, Orientation Image Microscopy (OIM) is applied to determine the crystallographic grain orientation within a selected area of approximately 200x200μm. OIM permits two thousands of orientation measurements per hour; hereby a given region of a specimen is photographed in the SEM at two different loading stages. A digital image processing system has been developed to find homologue points on the two photographs. Between 15.000 to 40.000 homologue points are detected within the specified area. The homologue points determine a deformation field that can be derived

numerically to obtain the local in-plane strain field. The variation of the grain orientations during each deformation step is measured by comparing the OIM analyses prior and after the deformation. The comparison yields maps where the rotation angle and the rotation axis are indicated. The crystallographic indices of the slip lines that are visible at the surface are evaluated. For each grain, the local deformations and the rotation angle are combined to estimate the active slip systems. This procedure is repeated for each deformation step. The experimental results are compared with predictions of a simplified Taylor model.

11:00 AM A1.7
FINITE ELEMENT SIMULATIONS OF THE DEFORMATION OF BCC AGGREGATES USING A CRYSTAL PLASTICITY MODEL IDENTIFIED AND VALIDATED ON SINGLE CRYSTAL EXPERIMENTS. STUDY OF LOCAL ORIENTATION EFFECTS.
David Arizmendi, LPMTM, Université Paris-Nord, Villetaneuse, FRANCE; Jean L. Raphanel, LMS, Ecole polytechnique, Palaiseau, FRANCE.

One considers b.c.c. iron at room temperature and low strain rates. The mechanisms of plastic deformation are crystallographic glide on two families of slip systems : $\{110\} < 111 >$ and $\{112\} < 111 >$, with initial asymmetry of glide for the {112} planes. The behavior of the single crystals is then intermediate between the behaviors at low and high temperature. One may thus express a critical shear stress on a slip system as a sum of an effective shear depending on strain rate and temperature, and an athermal shear, proportional to the square root of the sum of dislocation densities weighed by the coefficients of an interaction matrix. The evolutions of the dislocation densities are then related to the slip rates.
The parameters of these constitutive and hardening relations have been identified on single crystal tensile tests from the literature. The model is then implemented in a finite element code and validated on specific single crystal experiments.
An aggregate in the shape of a tensile specimen has then been designed. It is made of few grains of well-known geometry and initial orientations. One performs several simulations, keeping the same crystallographic texture, but varying the location assigned to a few crystallites. The aim is to assess, among other features of the plastic response, the importance of a local orientation distribution on the global behavior. While one arrangement of orientations yields an almost homogeneous state of deformation, another leads to an almost localized behavior. These two different behaviors would have been predicted as the same by classic micro-macro approaches (Taylor, self-consistent,...) since these models only account for crystallographic textures and not for local orientation distributions.
In this one instance, the interest of finite element simulations using crystalline plasticity for investigating local effects in the behavior of polycrystalline aggregates has been shown.

11:15 AM A1.8
ORIENTATION EFFECTS ON SHEAR LOCALIZATION IN Ti-6Al-4V.
Scott E. Schoenfeld, Army Research Lab, APG, MD; Bimal Kad, U.C. San Diego, Dept. of AMES, La Jolla, CA.

The goal of the current work is to examine the influence of crystallographic texture on plastic flow during high-strain-rate shearing of Ti-6Al-4V. A continuum model for the Ti-6Al-4V aggregate will begin by implementing the two-dimensional kinematic approximation to the hexagonal close-packed (hcp) crystal structure first proposed by Kad et al. (1995) for TiAl single crystals. The resistance to slip motion on this structure will follow the description used to model isotropic polycrystalline Ti-6Al-4V during impact events (Johnson, 1986) and will be implemented using the high-rate integration scheme proposed by Schoenfeld (1997). The resulting constitutive theory has been implemented into an explicit Eulerian numerical scheme (Benson, 1995) in order to solve the boundary-value problem of an aggregate of single crystals subject to simple shearing at high strain-rates. The effects of various thermo-mechanical processing will be assessed via the incorporation of different orientation distributions of the single crystals, and observations of shear band phenomenology (shear band path and directions) will be correlated with the ability of the aggregate to absorb energy within the high-rate environment. To the extent that such simple shear can be used to approximate the predominant failure mode (shear plugging; Burkins et al., 1997) during ballistic limit testing, our model will guide the development of subsequent thermo-mechanical processing of ballistic resistant Ti.

11:30 AM A1.9
DISLOCATION RELATED MODELING OF STRESS RELAXATION IN SUPERALLOYS.
Ulrich Martin, Uwe Muehle, Heinrich Oettel, Institute of Physical Metallurgy, Freiberg University of Mining and Technology, Freiberg, GERMANY.

Relaxation of residual stresses in metallic materials is caused by diffusion of inhomogeneously distributed solved alloying elements and by microstructural mechanisms like rearrangements of dislocation structure and precipitation processes, respectively. These processes are often linked with each other. Therefore, the description and the modeling of stress relaxation on a microstructural basis is often very complicated. The present study describes the application of hot deformation experiments and microstructure investigations in order to predict the relaxation behaviour of the highly loaded superalloys $NiCr_{22}Co_{12}Mo_9$ and $CoCr_{22}Ni_{22}W_{14}$. The results of mechanical tests and transmission electron microscopy (TEM) investigations have been used as input data into two models (an effective stress model and a modified constitutive model by Kocks-Mecking), which describe the relaxation of tensile loading stresses. It is the aim of the microstructure investigations to estimate parameters like dislocation density and carbide spacing for a dislocation related modeling using these two models. In stress relaxation tests the microstructure development was connected with a rearrangement of dislocation structures and a decreasing dislocation density. The stress relaxation in carbide strengthened superalloys is a typical case of dislocation relaxation in the presence of precipitates. By including the estimated microstructure parameters, the simulation of relaxation behaviour by these two models yields results which accurately predicts the tensile and relaxation behaviour.
References: U. Muehle, U. Martin, H. Oettel, O. Voehringer, Mat. Sci. Eng. A230 (1997) 81-87; U. Martin, H. Oettel, U. Muehle, Stress Relaxation in Superalloys Due to Microstructural Changes, Mechanics of Time-Dependent Materials 2 (1998), 1-12

SESSION A2: NONLOCAL PLASTICITY THEORY AND DISLOCATION PHENOMENA
Chairs: Huajian Gao and David H. Lassila
Tuesday Afternoon, November 30, 1999
Room 208 (H)

1:30 PM A2.1
STRAIN GRADIENT EFFECTS IN BENDING.
John Y. Shu, Engineering Department and James S. Stölken, Chemistry and Materials Science Directorate, Lawrence Livermore National Laboratory, Livermore, CA.

A strain gradient crystal plasticity formulation (Shu and Fleck, 1999) is applied to study the bending of thin metal sheets. A microbend experiment (Stolken and Evans, 1998) has shown that the normalized bending moment exhibits a significant dependence on the thickness of the sheet which is not accounted for within the classical plasticity framework. The strain gradient crystal formulation takes into account the extra hardening effect of the spatial gradient of crystal slip on slip resistance and length scales thus enter the constitutive law and provide the bases of scale-dependent predictions. The finite element method model consists of a chain of single crystal grains under plane strain deformation. Both uniformly and randomly distributed crystal orientations are considered. The normalized bending moment thus predicted is found to exhibit a strong dependence on the thickness. The length scales pertaining to crystal slip systems are inferred by comparing the finite element results with the experimental measurement and are found to be in the range of a few microns.
Shu, J.Y. and Fleck, N.A. (1999) J. Mech. Phys. Solids 47, 297-324. Stolken, J.S. and Evans, A.G. (1998) Acta metall. 46, 5109-5115.
This work is performed under the auspices of U.S. Department of Energy and Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

1:45 PM A2.2
A STUDY OF MICRO-INDENTATION AND NANO-INDENTATION HARDNESS TESTS BY MECHANISM- BASED STRAIN GRADIENT PLASTICITY.
Y. Huang, Z. Xue, Univ of Illinois, Dept of Mechanical Engr, Urbana, IL; H. Gao, Stanford Univ, Div of Mechanics and Computation, Palo Alto, CA; Z.C. Xia, Ford Research Lab, Dearborn, MI.

We have recently proposed a theory of mechanism-based strain gradient (MSG) plasticity to account for the size dependence of plastic deformation at micron and submicron length scales. The MSG plasticity theory connects micron scale plasticity to dislocation theories via a multiscale, hierarchical framework linking Taylor's dislocation hardening model to strain gradient plasticity. The motivation for developing such a theory has come from our previous analysis of micro-indentation experiments, which strongly suggest a linear dependence of the square of plastic flow stress on strain gradient. Here we show that the theory of MSG plasticity, when used to study micro-indentation, indeed reproduces the linear dependence observed in experiments, thus providing an important self-consistent check of the theory. In accomplishing this objective, we have generalized the MSG plasticity theory to including the elastic deformation in the hierarchical framework. Some modifications to the

length scale in MSG plasticity are also discussed. These include the Taylor factor which relates the tensile yield strength to the critical resolved shear strength for crystalline materials and the Nye factor which calibrates the scalar measure of geometrically necessary dislocation density from macroscopic plastic strain gradients.

2:00 PM A2.3
EFFECT OF PRECIPITATE MORPHOLOGY ON THE GRADIENT-DEPENDENT BEHAVIOUR OF TWO-PHASE SINGLE CRYSTALS. Esteban P. Busso, Franck T. Meissonnier, and Noel P. O'Dowd, Department of Mechanical Engineering, Imperial College, London, UNITED KINGDOM.

During high temperature deformation of single crystal superalloys, the initially cuboidal precipitates undergo morphological and volume fraction changes which strongly affect the single crystal mechanical properties. In this work, the combined effects of the precipitate morphology and slip gradients which develop near the precipitate interfaces due to local deformation incompatibilities are investigated using a micro-macro continuum mechanics approach. A recently proposed dislocation mechanics-based rate and gradient dependent crystallographic formulation [1][2] is used to describe the behaviour of the soft matrix of a precipitated single crystal. It relies on strain gradient concepts to account for the additional strengthening mechanism caused by presence of interfacial and geometrically necessary dislocations (GNDs). The total slip resistance is assumed to be due to a mixed population of mobile and sessile forest obstacles arising from both statistically stored (SSDs) and GNDs. Details about the numerical implementation of the non-local crystallographic theory into the finite element method will be presented. This includes the calculation of the slip rate gradients at the element level to determine the evolutionary behaviour of the GND densities, and a fully-implicit numerical algorithm within a large strain kinematics framework to update the local stresses and internal slip system variables [3]. Results from 3D unit cell type computations are compared with $< 100 >$ uniaxial data and discussed vis-a-vis the predicted spatial gradients of inelastic strains and distributions of SSDs and GNDs within the soft matrix channels. The effects of the precipitate morphology (including directional coarsening), size and volume fraction on the macroscopic stress-strain response of the precipitated single crystal are also investigated.
References:
[1] E.P. Busso and F.A. McClintock, Int. Journal of Plasticity, V. 12, pp. 1-28 (1996).
[2] E.P. Busso, F.T. Meissonnier and N.P. O'Dowd, Journal Mech. Phys. Solids (1999). (Submitted).
[3] F.T. Meissonnier, E.P. Busso and N.P. O'Dowd, Int. Journal of Plasticity (1999). (Submitted).

2:15 PM A2.4
EXPERIMENTAL ANALYSIS AND CRYSTALLOGRAPHIC MODEL OF THE LOCALIZATION OF PLASTIC DEFORMATION AFTER A CHANGE OF LOADING PATHS IN MILD STEEL POLYCRYSTALS. Thierry Hoc, Colette Rey, Ecole Centrale Paris, Dept Mecanique Sols, Structures et Materiaux, Chatenay, FRANCE.

In polycrystals, localization of the plastic deformation during metal forming processes, is considered as the result of large deformations and (or) the result of change of loading paths. Such heterogeneous deformation increases the ductility then leads to rupture. In order to determine, the mechanisms ruling the localization of mild steel polycrystals, two changes of loading paths are performed, corresponding to a plane tension followed by parallel and orthogonal uniaxial tension. The localization phenomena is analysed at macroscopic, mesoscopic and microscopic scales thanks to different techniques such as local texture (EBSD) and microextensometry by microgrids. SEM observations and local strain field computations pointed out that macrobands of localization propagate by activation of two families of short parallel coarse slip bands. This experimental background, added to the observations of the microstructure of dislocations suggests that bifurcation is bound to the anisotropy of the microstructure. By contrast, the post-bifurcation may be correlated to a textural and a microstructural softening allowing large localized strains without increase of the density of dislocations. A simulation of the localization process based on the Finite Element Method is proposed. The polycrystal is constituted by a real pattern of 114 grains six times juxtaposed. The constitutive law is a viscoplastique power law based on a hardening matrix whose terms depend on the densities of dislocations on each slip systems. Such a model allows in one hand, to represent the anisotropy and evolution of the microstructure of dislocations and in other hand to get large strains and staturations of the density of dislocations. The results of the simulation is an accurate description of the localization within the grains of the polycrystal as a function of the orientation of the second path loading and the rate of the prestrain.

3:00 PM *A2.5
COMPLEMENTARY EXPERIMENTAL TECHNIQUES FOR MULTI-SCALE MODELING OF PLASTICITY. Lyle Levine and Gabrielle Long, Materials Science & Engineering Laboratory, National Institute of Standards and Technology, Gaithersburg, MD.

The recent expansion taking place in the fundamental science of plasticity has been driven primarily by the revolution in computer hardware and the subsequent development of dislocation dynamics codes that simulate the behavior of many interacting dislocations in three dimensions. New theoretical advances are also taking place, mostly based upon modern developments in statistical physics. Unfortunately, progress in these areas is being hampered by a paucity of experimental data on key facets of dislocation structure evolution. Such data is required both as a guide to the development of theoretical and computational models as well as the ultimate test of their validity. Some recently-developed experimental techniques, such as *in situ* ultra-small-angle X-ray scattering (USAXS), have demonstrated a capability for measuring aspects of dislocation structure evolution that are inaccessible to other experimental methods. However, no single technique can provide the entire range of information required by theoretical and computational researchers. It is only through the synergy of several experimental techniques (including USAXS, transmission electron microscopy, diffraction-peak profiling, micro-mechanical testing, diffraction imaging, orientation imaging microscopy, etc.) that much of the required data can be obtained. Ultimately, the development of additional new experimental techniques will also be required. Work in all of these areas is ongoing, and current combined experimental efforts involving many of the necessary techniques are underway. Such collaborative work will be the primary focus of this talk.

3:30 PM A2.6
UNRAVELING MICROSTRUCTURAL FEATURES AND PROCESSES IN POLYCRYSTALLINE METALS THROUGH THE SYNTHESIS OF EXPERIMENTAL, THEORETICAL, AND COMPUTATIONAL APPROACHES. C.R. Myers, Cornell Theory Center; E. Muller, A. Mathur, J.P. Sethna, Laboratory of Atomic and Solid State Physics; T.J. Turner, M.P. Miller, P.R. Dawson, Sibley School of Mechanical and Aerospace Engineering; S.R. Arwade, E. Iesulauro, C.-S. Chen, A.R. Ingraffea, School of Civil and Environmental Engineering; Cornell University, Ithaca, NY.

Microstructural aspects of polycrystalline metals continue to be better understood due to advances in experimental techniques, computational capabilities, and theoretical analyses. Improved understanding of both statistical characterizations – such as orientation and misorientation distribution functions – and specific structural features – such as dislocation cells and microcracks – will ultimately enable more accurate materials predictions through the use of multiscale modeling techniques. Such techniques will allow for more fundamental information from smaller scales to be judiciously folded into larger scale computations, either through the use of improved constitutive descriptions or through explicit representation and simulation at multiple scales. We are combining techniques on several fronts to better understand the nature of polycrystal plasticity, the formation and evolution of subgrain deformation structures, and the relationships between local misorientation and microcrack formation. Our approach combines automated experimental imaging techniques (electron backscatter diffraction), experimental testing (fatigue), simulation techniques (finite element methods for polycrystal plasticity), and various theoretical methods (scaling analyses, order parameters and group theory). For example, detailed analyses of the spatial structure of orientation data from EBSP scans and FEM simulations can assist us in the development and testing of models of dislocation structure formation, or of microcrack initiation. We are building tools to connect and explore these complementary approaches under the umbrella of our Digital Material, a modeling and software framework to facilitate multiscale, multidisciplinary descriptions of material deformation and failure.

3:45 PM *A2.7
IN-SITU TRANSMISSION ELECTRON MICROSCOPY STUDIES OF DISLOCATIONS IN THIN FILM SYSTEMS. Eric A. Stach, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA; R. Hull, Department of Materials Science, University of Virginia, Charlottesville, VA; R.M. Tromp, F.M. Ross, K.W. Schwarz and M.C. Reuter, Research Division, IBM T.J. Watson Research Center, Yorktown Heights, NY; W.D. Nix and J. Florando, Department of Materials Science, Stanford University, Palo Alto, CA.

In-situ transmission electron microscopy of thin films systems provides an ideal experimental laboratory for the study of dislocation motion and dislocation - defect interactions in materials. Through careful consideration of the sample geometry and calibration of the experimental conditions it is possible to obtain accurate quantitative information about dislocation velocities, interaction stresses and

overall strain relaxation behavior. A model materials system for studies of dislocation behavior is heteroepitaxial SiGe layers grown on Si substrates. In this case the difference in lattice parameter between the layers results in mismatch strains and stresses whose magnitude can be directly controlled by the choice of germanium concentration and sample thickness. During growth and annealing within the microscope, dislocations nucleate and grow in order to relieve this mismatch strain. Quantitative observations of the interaction between moving threading dislocations and other interfacial misfit dislocations will be presented. These observations are amenable to direct comparison with mesoscale modeling of dislocation dynamics, and we will discuss in particular the interplay between experimental observation and computational modeling that has lead to understanding of the important phenomenon of reactive blocking in heteroepitaxial strain relaxation. Additionally, it is possible to use thermal mismatch strains to move dislocations through thin films. Results from in-situ thermal cycling of sputter-deposited aluminum films grown on silicon-on-insulator wafers will also be discussed. Use of selective etching techniques permits observation of free standing Al/Si layers in-situ, allowing one to identify the dislocation mechanisms that control strain relaxation in these films. These observations can be correlated with direct measurements of strain relaxation made by wafer curvature and bulge testing techniques, providing an important cross-link with other experimental methods of studying dislocation-based strain relaxation.

4:15 PM A2.8
SURFACE FILM SOFTENING EXPERIMENTS AS INPUT FOR MODELING OF DEFORMATION AND FRACTURE.
Ronald Gibala, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI and Sandia National Laboratories, Livermore, CA.

The phenomenon of surface film softening is observed in several classes of dislocation mobility limited or dislocation density limited materials. The purpose of this talk is to demonstrate its usefulness as input data for testing predictions of various methods of modeling crystal plasticity, dislocation dynamics, and fracture behavior of materials. Surface film softening is manifested as enhanced plasticities and/or reduced flow stresses in film coated materials relative to that of the uncoated substrates. It has been observed in body centered cubic metals, B2 ordered compounds and tetragonal silicides in tension, compression, fatigue and indentation experiments. Some of the basic experiments are reviewed. Implications for the analysis and modeling of multi-scale deformation and fracture phenomena, as well as ideas for new experiments, are suggested.

4:30 PM A2.9
SIMULATION OF DISLOCATION MOTION IN CONFINED GEOMETRY UNDER NONUNIFORM STRESS FIELD.
C. Lemarchand, DMSE, ONERA, Chatillon Cedex, FRANCE; B. Devincre, L. Kubin, LEM, CNRS-ONERA, Chatillon Cedex, FRANCE; J.L. Chaboche, DMSE, Chatillon Cedex, FRANCE.

In order to describe the plastic behavior of crystalline materials containing structural heterogeneities and/or under complex loading, a new non local method that incorporates both dislocation properties and a rigorous treatment of the boundary value problem is proposed. This new computer model involves the coupling of two different types of three-dimensional simulations: a Finite Elements code and a Dislocation Dynamics simulation at the mesoscopic scale. The basics of this new computer model are presented and its potentialities are illustrated by results on the onset of plastic flow in thin films. Comparisons are made between previous calculations of threading dislocations in metallic films and the present computer model predictions.

4:45 PM A2.10
DISLOCATION MULTIPLICATION AND STRAIN HARDENING IN BCC SINGLE CRYSTALS: 3D DISLOCATION DYNAMICS SIMULATIONS.
Meijie Tang, Physics Directorate, Lawrence Livermore National Lab., Livermore, CA; Benoit Devincre, Ladislas P. Kubin, LEM, CNRS-ONERA, Chatillon, FRANCE.

A previously developed dislocation dynamics simulation method is used to study the dislocation multiplication and strain hardening of BCC single crystals at low temperatures. Due to the strong anisotropy in the mobilities of the screw and edge dislocations, the dislocations multiply signficantly during the initial stage 0 plastic deformation, which occurs before the actual yielding takes place. At the end of the stage 0, the dislocation density can increase by an order of magnitude and elongated screw dislocations on all slip planes will participate in subsequent strain hardening. The dislocation dynamics simulation is used to investigate the dislocation multiplication and its dependence on the initial dislocation structures, such as the average dislocation length, initial density, and the simulation volume size. The objective is to understand the characteristics of dislocation multiplications. The later combined with the forest hardening studied earlier will lead to the strain hardening of BCC crystals at low temperatures.
Supported by U.S. DOE under contract No. W-7405-ENG-48

SESSION A3: POSTER SESSION: MULTI-SCALE PHENOMENA IN CRYSTAL PLASTICITY

Chairs: Young Huang and James S. Stolken
Tuesday Evening, November 30, 1999
8:00 P.M.
Exhibition Hall D (H)

A3.1
MODELING THERMALLY ACTIVATED INELASTIC DEFORMATION WITH CELLULAR AUTOMATA.
Glenn S. Daehn, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH.

Traditional models of plastic deformation implicitly assume dislocations (with a uniform, fixed stress acting upon them) attempt to overcome obstacles of a single characteristic size and shape. This results in models that lend themselves to closed-form analysis. Here models of thermally activated inelastic flow are developed based on a probabilistic cellular automata framework. The defining characteristics of the models are: a range of obstacle strengths is specified and these are randomly distributed spatially; obstacles are overcome in a probabilistic way based the strength of the obstacle, local stress and temperature; the stress on a given obstacle is related to the relative strain states of it and its near neighbors (such that the average stress is constant). It will be shown that such models very naturally produce the characteristics observed in creep transients, including classical creep transients and anelastic backflow. The role of such models in interpreting experimental observations will be emphasized.

A3.2
SYNCHROSHEAR VERSUS CONVENTIONAL SHEAR MECHANISMS IN TRANSITION-METAL DISILICIDES WITH THE C40 STRUCTURE.
H. Inui and M. Yamaguchi, Dept. Materials Science & Engineering, Kyoto University, Sakyo-ku, Kyoto, JAPAN.

There is a growing interest in transition-metal disilicides as possible candidates for very-high-temperature structural applications. These disilicides include $MoSi_2$ and WSi_2 with the tetragonal $C11_b$ structure, VSi_2, $CrSi_2$, $NbSi_2$ and $TaSi_2$ with the hexagonal C40 structure and $TiSi_2$ with the orthorhombic C54 structure. The generation of the three different structures is accomplished by changing the stacking order of the $MeSi_2$ layers; these three structures are based on the AB, ABC and ADBC stacking sequences, respectively. Thus, $\{110\} < 111]$ slip in the $C11_b$ structure, $(0001) < 11\bar{2}0 >$ slip in the C40 structure and $(001)[110]$ slip in the C54 structure are all equivalent. We have investigated the plastic deformation behavior of the equivalent slip systems of the three different structures, using single crystals of these transition-metal disilicides. The onset temperature for plastic flow for the equivalent slip systems as well as their CRSS value vary from silicide to silicide. However, when the CRSS and temperature are normalized respectively to the shear modulus and melting temperature, the normalized CRSS-temperature plot indicates that these disilicides are classified into two groups regardless of crystal structure. One group consists of $MoSi_2$, VSi_2, $NbSi_2$, $TaSi_2$ and $TiSi_2$ and exhibits an onset temperature for plastic flow at around 0.3 the melting temperature. The other group consists of $CrSi_2$ and $Mo(Si,Al)_2$, both of which have the C40 structure, and exhibits an onset temperature for plastic flow at around 0.6 the melting temperature. High-resolution transmission electron microscopy of dislocation core structures indicates that while silicides of the former group deform by a conventional single shearing mechanism, those of the latter group deform by a synchroshear mechanism, in which a sequence of shears occur on two adjacent slip planes. Factors controlling the operation of the synchroshear mechanism will be discussed in terms of the nature of atomic bonding in transition-metal disilicides.

A3.3
THE NATURE OF MECHANICAL PROPERTIES OF SINGLE-CRYSTAL AND NANOCRYSTALLINE ALLOYS.
Valery P. Kisel, Institute of Solid State Physics, Chernogolovka, Moscow, RUSSIA.

The remarkable finding of this work is the identical correlation between the starting stresses of various stages of plastic flow or fracture at different scale lengths of observations (atomic,micro-, meso- and macroscopic scales [1]), and the starting stresses for the first microcrack or macrocrack nucleations in single and polycrystalline alkali halides, disordered alloys, semiconductors and superconductors, ceramics. The experimental data prove that this scaling is universal for the widest temperature, stress and stress rate

ranges (up to the shock stresses), for the materials with various volume fraction and impurity state, precursor strain and thermal prehistory, etc. This universal scaling of stresses points to the controlling role of deformation stress and to the same micromechanisms of plasticity in the strict chain of deformation modes: dislocation motion and multiplication, dislocation cross-slip, climb and full stop, the grain boundary origin, polycrystalline-nanocrystalline and amorphous state, the first microcracks nucleation, then their coalescence into macrocracks (macrofracture) and the formation of fracture surfaces. Structural investigations and literature data confirm this sequence of the deformation modes. Due to different properties of dislocation double cross-slip, climb and the Orowan bowing under various types of loadings (shock, impact, Instron or creep) the dislocation structure nearby the crack tips, the corresponding fracture modes (so called ductile, brittle or cleavage ones) and the structures of rupture surfaces differ to a great extent from each other. [1] V.P. Kisel, Mater. Sci. Engn., 1993, 164A, p. 356. [2] V.P. Kisel, Proc. of ISMA-9, Haifa, 1, 601 (1991).

A3.4
SURFACE INSTABILITIES AND PLASTIC DEFORMATION OF COPPER/TANTALUM CYLINDRICAL CONDUCTORS. J. Colin, J. Grilhé, Université de Poitiers, Laboratoire de Métallurgie Physique, SP2MI Futuroscope, FRANCE; L. Thilly, F. Lecouturier, S. Askénazy, Service National des Champs Magnétiques Pulsés, CNRS UPS INSA Toulouse, FRANCE; J.P. Peyrade, Laboratoire de Physique de la Matiere Condensee, CNRS UPS INSA, Toulouse, FRANCE.

When a solid is submitted to non-hydrostatic stresses, sinusoidal fluctuations of its surface can appear and develop by diffusion to relax the stored elastic energy: this is the Asaro-Tiller-Grinfeld instabilities. The formalism of Asaro-Tiller-Grinfeld instabilities has been used to model the development of two set of surface instabilities which have been observed during the elaboration of copper/tantalum cylindrical conductors under stress. Axial and radial sinusoidal fluctuations have been introduced simultaneously on the cylindrical surface of a stressed conductor. The stress relaxation has been calculated and an energy variation calculation has been performed to determine the theoretical wavelengths of these oscillations. A study of the cylinder surface kinetics has been then performed to characterize the evolution of the roughness versus time. The different results are compared to the experimental observations of the interface of copper/tantalum conductors.

A3.5
EFFECTS OF MATERIAL INHOMOGENEITY AND ANISOTROPY ON SERRATED PLASTIC FLOWS. Xianghong Li, Wei Tong, Yale University, Dept. of Mechanical Engineering, New Haven, CT.

Serrated or unstable plastic flows due to dynamic strain aging of dislocations have been observed in both AA5XXX and AA6XXX aluminum sheet metal alloys. A dislocation-based viscoplastic model is formulated to account for the interaction between dislocations and alloying atoms over a range of length and time scales. The proposed model is implemented in a finite element program to simulate the unstable plastic flows in aluminum sheet metals. Special attention is paid to the materials with both planar mesoscale inhomogeneity and/or anisotropy and their effects on the spatial-temporal characteristics of the unstable flows. The study aims to identify the possible dominant mechanisms that distinguish the plastic behavior between the AA5XXX and AA6XXX aluminum alloys.

A3.6
A MODEL FOR CALCULATING SUBSTRATE CURVATURE DURING COALESCENCE OF Pt ISLANDS ON AN AMORPHOUS SUBSTRATE. Mark A. Phillips, Vidya Ramaswamy, Bruce M. Clemens, William D. Nix, Stanford University, Dept of Materials Science and Engineering, Stanford, CA.

Understanding the relationship between film stress and the corresponding microstructure at various stages of growth allows accurate prediction and control of film microstructure. Previous work involving in-situ stress measurement and ex-situ microstructural characterization has shown a correlation between stress and microstructure during the early stages of growth. The model presented here can be used to predict stress during part of this growth process. Stress is measured in-situ during growth of sputter-deposited Pt on amorphous substrates. The film stress is observed to be slightly compressive at nominal thicknesses less than 10 $\AA$, followed by a change towards a tensile maximum at 30 $\AA$, after which the stress becomes compressive again. Plan view TEM micrographs of Pt films of thicknesses ranging from 3 $\AA$ to 35 $\AA$ show the evolution of microstructure from isolated islands to a coalesced film. This evidence suggests that the tensile regime is due to film coalescence by the spontaneous snapping together of individual islands, and the tensile maximum then marks the completion of coalescence. This study presents a simple model to calculate the curvature induced in a substrate during the tensile excursion associated with island coalescence, where discontinuous islands are modeled as a series of cracks in an otherwise continuous film. Quantitative information such as feature size, size distribution and island density is extracted from the TEM micrographs and the model is used to calculate the magnitude of tensile stress generated during coalescence. The predicted stress is compared to the measured in-situ stress.

A3.7
ATOMIC-SCALE DESIGN FOR ENHANCED LOW TEMPERATURE TWINNING IN $ZrCr_2$-BASED LAVES PHASES. Won-Yong Kim, David E. Luzzi, Univ of Pennsylvania, Dept of Materials Science and Engineering, Philadelphia, PA.

The Laves phases are viewed as potential high temperature structural materials due to the existence of phases with high melting temperatures, excellent strength and creep properties, and good oxidation resistance. However, the technological application of these materials is restricted by brittle fracture behavior at low temperatures. Recently, we have designed and produced several transition metal Laves phases with low-temperature compressive ductility. These improved alloys demonstrate that manipulation of atomic-scale structure can have a drastic effect on meso-scale deformation behavior. To gain a basic understanding of the role of atomic-scale substitutions on the room temperature mechanical properties, a systematic investigation of the C15 $ZrCr_2$-based alloy system was conducted and is reported here. Compression tests were carried out on ternary Zr-Cr-X(X = Hf, Ti, Nb, Ta) alloys of various compositions. The flow behavior by twinning is found to be markedly different as a function of the alloying element. The results, including x-ray diffraction and transmission electron microscopy analyses, will be discussed with respect to the relative importance of atomic size and electronic structure on twinning in these C15 Laves phase-based alloys.

A3.8
MEASUREMENT OF CRACK VELOCITY IN ICE WITH HIGH-SPEED PHOTOGRAPHY, ACOUSTIC EMISSION, AND RESISTANCE METHOD. Patrick Donovan, Victor F. Petrenko, Dartmouth College, Thayer School of Engineering, Hanover, NH; Masahiko Arakawa, Norikazu Maeno, Hokkaido University, Instutute of Low Temperature Science, Sapporo, JAPAN.

Measurements of crack velocity in ice using electric-resistance method showed one-to-two order of magnitude difference in crack velocity for freshwater and saline ice [1] while recent experiments in which high-speed photography was used didnt confirm that result [2]. Different types of ice and loading modes were used in the cited papers. To resolved the contradiction we performed simultaneous measurements of crack velocity in different ices and in wide temperature range of ~5C to ~40C using several common techniques: high-speed photography (up to one million frames per second), electrical resistance method, acoustic emission method, and crack opening measurements. Columnar freshwater and saline ices were used. Double-cantilever beam fracture test geometry was used to initiate cracks. We found that the high-speed photography in which cracks were observed under total internal reflection condition was the most reliable technique capable to reveal very thin (micrometer-thick) cracks. Indeed, we confirmed that the crack velocity in saline ice containing unfrozen liquid inclusions was lower than that in freshwater ice. Though, the difference between two ices was smaller than it was found using the electric-resistance method. The records of acoustic emission were difficult to use to determine crack velocity. Crack opening signals were detectable only after cracks cut entire ice samples. 1. Petrenko, V. F. and Gluschenkov, O. (1996) Crack velocities in freshwater and saline ice. J. Geophysical Research., 101(B5): 11541. 2. Arakawa, M., Petrenko, V.F. and Maeno, N. (1998) Propagation of cracks in ice with liquid inclusions. Proc. of the 1998 Annual Meeting of Japanese Society of Snow and Ice, p.44.

A3.9
STRESS AND TEMPERATURE DEPENDENCE OF Ga PENETRATION RATES IN A HIGH STRENGTH Al ALLOY. Boxiong Ding, Richard G. Hoagland, Kelvin G. Lynn, Washington State University, Materials Science Program, Pullman, WA.

Penetration of Gallium on grain boundaries in aluminum and its alloys strongly depends on stress. This behavior suggests a potential method to measure residual stress in aluminum parts. The penetration of Ga in Al alloys 7050 T74 and 7050 T7451 with and without applied stress has been studied. The temperature dependence of the penetration velocity was measured to obtain the activation energy for both conditions and for pure Al. These results suggest a possible rate controlling mechanism for this phenomenon. Crack growth experiments on compact tension specimens show that the crack growth rate exponentially depends on the stress intensity factor.

SEM observation of the penetration of Ga on the grain boundaries are also reported. This research is supported by DARPA/NRL under Grant N00014-97-1-G007.

A3.10
CRITICAL GROWTH OF FRACTAL FATIGUE DEFECTS.
Marek Rybaczuk, Wroclaw Univ of Technology, Institute of Matls Science & Applied Mechanics, Wroclaw, POLAND.

Material defects growing during fatigue or damage process are described in terms of fractals. The assumed, uniform energy distribution over fractal defects corresponds to generalized energy density, treated as material characteristics. It has been shown that the way of evolution as well as the main features of an irreversible process are determined by characteristic (for a given material) fractal measures. The defects localization runs in accordance with characteristics measures and remains proportional for finite characteristics measures. The macroscopic range of length scales has been introduced via additional energy dependence upon macroscopic volume limiting defects evolution. The involved parameter determines the Hausdorff distance from defects structure to the macroscopic range of scales. Under certain constrains imposed upon defects growth, the effect similar to phase transition can be observed. The transition point coincides with the singularity of characteristic measures. In turn, the singularity comes from macroscopic limitations of defects growth. Theoretical results are compared with numerical simulations of the simplified stochastic fibre break process in composites. The simplified model has been generated in a way allowing to exclude heat outflow from the simulated system. This makes possible to examine defects growth over full range of scales beginning with the microscopic level. The calculated singularity appears at percolation point when observed correlated defects approach macroscopic size in accordance with the proposed theoretical model. The similar behavior follows from relative partition entropy considerations. The stable state (free energy extreme) coincides with characteristic measures. It has been also shown that the energy flow always runs from (the longest) macroscopic range of scales towards (the shortest) microscopic scales unless the additional entropy sources are involved. Theoretical concepts are compared with experimental tests for steels what enables to determine range of length scales corresponding to characteristics measures as well as the irreversible fatigue evolution threshold.

A3.11
LONG DISTANCE FRACTURE SURFACE ROUGHNESS ON A DENDRITIC ALUMINUM ALLOY.
J. Aldaco, F.J. Garza, M. Hinojosa, Facultad de Ingenieria Mecanica y Electrica, Universidad Autonoma de Nuevo Leon, San Nicolas de los Garza, Nuevo Leon, MEXICO.

The long distance roughness of the fracture surface of a dendritic aluminum alloy is studied over a wide range of length scales. Self-affinity analysis was performed over samples broken in Charpy impact tests. Simultaneous use of Atomic Force Microscopy, SEM and stylus profilometry allowed us to cover a wide spectrum of legth scales, spanning over seven decades, from a few nanometers up to one centimeter. The roughness exponent and correlation length were obtained using the variable bandwidth and the power spectrum methods. For the roughness exponent, a value of 0.8 was recovered, corresponding to the reported universal exponent. Correlation length was found to correspond well to the characteristic length of the largest heterogeneities in the complex microstructure. Our results provides information that can help to improve our understanding of the role of microstructural parameters on crack propagation mechanisms.

A3.12
EXPERIMENTAL OBSERVATIONS OF INDENTATION SIZE EFFECTS IN GOLD THIN FILMS.
Erica T. Lilleodden, William D. Nix, Stanford University, Dept of Materials Science & Engineering, Stanford, CA.

Indentation is an obvious experimental technique for exploring the predictions of multi-scale modeling because it spans all of the relevant length scales. It has been shown that experimental observations of indentation size effects may be understood in terms of strain gradients, but strain gradient models maintain a continuum framework and cannot be expected to explain anomalous behavior at the nanometer scale. In particular, observations of load-displacement discontinuities in the initial stages of indentation imply that dislocation nucleation occurs. Atomistic simulations of idealized indentation configurations have shown that surface nucleation of dislocation loops occur at near-theoretical shear strengths. Such studies have provided a basis for comparison of experimental observations, but simulations of realistic indentations are not yet available. Experimental observations of discretized indentation behavior in $< 111 >$ oriented films will be described in terms of both dislocation nucleation events and strain gradient plasticity. FEM simulations have been used to extract the effective yield strengths at 'stable' points along the experimental load-displacement curves, and results are compared to the depth dependent hardness computed by both the Oliver-Pharr method and a method in which the contact area is determined directly by a Sneddon analysis. Although the FEM results correspond reasonably well with the Oliver-Pharr hardness, a large discrepancy exists with the results based on Sneddon's analysis. The exceptionally high hardnesses calculated using the Sneddon equation is explained in terms of a constant contact area during dislocation emission. Additionally, it is shown that the observed hardness-displacement relationships deviate from the strain gradient model prediction due to the non-continuum mechanisms of deformation which dominate at indentation depths less than 50nm.

A3.13
STOCHASTIC MESOSCALE MODELING OF ELASTIC-PLASTIC DEFORMATION.
Alexander Staroselsky, United Technologies Research Center, East Hartford, CT; and Vasily V. Bulatov, Lawrence Livermore National Laboratory, Livermore CA.

Plastic response of a solid under stress depends on its crystallographic structure and morphology. Two major mechanisms of plasticity in metals are crystallographic slip and twinning. The purpose of this work is to analyze the influence of local stress distribution on slip and twin nucleation and propagation and to examine how this behavior depends on the interaction between slip and twin, between twin and twin, and between slip/twin and grain boundary. We formulate a simple model in which slip and twin systems are defined at appropriate angles to each other. Plastic flow is treated as a Markovian stochastic process consisting of a series of local inelastic transformations (LITs) in the representative volume elements (RVE). The probabilities of LITs per unit time are defined in the framework of transition-state theory. By varying the types of allowed LITs and/or the scale of RVE, plastic deformation is modeled at different structural levels, from a small volume of single crystal to the aggregate response of an isotropic polycrystalline solid. An important feature of this model is that evolution of the internal stress distribution is traced explicitly throughout the simulation run. This allows us to examine conditions of slip and twinning in considerable detail. In particular, we observe that twinning occurs through a nucleation-and-growth mechanism whose rate is controlled by the size of the critical nucleus of the new phase. We show that the model can be extended to incorporate several other realistic scenarios of deformation in polycrystals, including grain boundary irregularities, misfit energy, and inter-grain sliding.

A3.14
THE DETERMINATION OF EVOLVING MICROSTRUCTURE USING CONSTITUTIVE RELATIONSHIPS.
Brad J. Diak, Peter Poruks, Shig Saimoto, Department Materials & Metallurgical Engineering, Queen's University, Kingston, Ontario, CANADA.

The knowledge of the deformation microstructure in large part is derived from quasi-static testing of loading and unloading for structural change evaluation using electron metallography. From such studies considerable understanding of the origin of flow stress has been delineated but its evolutionary correlation to the measured stress-strain curve has been almost ignored. Our studies using high resolution load-inelastic deformation data show that the mean slip distance, $\lambda \equiv 0.5 b\mu^2 \div (\tau\ d\tau \div d\gamma)$, is functionally correct but the absolute magnitude is too high even at low temperatures where dynamic thermal recovery is negligible. The earlier work on dynamic resistivity measurement indicates that mechanical annihilation is possible even during Stage II suggesting that a quantitative relation between λ and Θ_{II} will result in a suitable proportionality factor. To examine the bases of this hypothesis, uniaxial tensile tests on nearly random oriented pure Al specimens of ultra-fine grain size (2-4 μm) were performed at various sub-ambient temperatures. The fine grain size which is stable at 230°C for 100 hrs. sets an upper limit to λ. By plotting λ versus flow stress, a minimum is observed which correlates well with published deformed cell size as a function of γ. However, during Stage III the principle of similitude is lost and λ increases with $\tau(\gamma)$ becoming multiples of the minimum cell size. As well, the maximum value near the ultimate stress does not exceed the measured grain size. The structure of the tangled walls can be simultaneously assessed by measuring the activation volume by precision strain rate sensitivity. Thus a dynamic quantitative measure of microstructure evolution appears possible which will be confirmed by spot measures of the cell size by transmission electron microscopy.

A3.15
Abstract Withdrawn.

SESSION A4: DISLOCATION DYNAMICS – EXPERIMENTS AND SIMULATIONS
Chairs: Marc C. Fivel and Yong-Qian Sun
Wednesday Morning, December 1, 1999
Room 208 (H)

8:15 AM *A4.1
3D DISCRETE DISLOCATION DYNAMICS : OVERVIEW AND LATEST DEVELOPMENTS. Marc C. Fivel, GPM2/CNRS, Grenoble, FRANCE.

The first 3D Discrete Dislocation Dynamics code was initiated by Kubin, Brechet and Canova in 1990. The idea was to develop a numerical model to understand the effect of the collective behavior of dislocations on the macroscopic response of a f.c.c crystal. The simulated entities are precisely the dislocation lines. The elastic dislocation theory is applied to each line and the global behavior is deduced from the collective interactions of all the elementary events. The model was chosen to be as simple as possible. The dislocation lines are discretized in a set of segments of pure edge or screw character. Those segments being perpendicular one to the other one, the motion of the set of segments describing a dislocation loop is made easier. The position of each dislocation segment is ascribed to a discrete lattice similar to the crystallographic network but larger so that the numerical code just deals with integers and the elastic theory is still available. Although very simple, such a method has proven to be very powerful to reproduce physical mechanisms such as plastic instabilities or work softening in f.c.c. alloys. More recently, the model has been used to understand the flow stress anomaly in $L1_2$ alloys (Devincre et al. 1997), to compute parameters involved in macroscopic behavior laws (Tabourot et al. 1997), and to simulate the nanoindentation test (Fivel and Robertson, 1998). Specific versions of the code have also been developed in order to deal with other crystallographic structures such as diamant cubic (Moulin et al., 1997 on silicon) and b.c.c. (Tang et al., 1998 on tantalum). All those codes can be seen as powerful tools which fills the gap between atomic methods and continuum mechanics.
After a brief description of the method, the present talk will illustrate its capability through several results obtained in the past few years. A special emphasis will be given on the latest developments achieved regarding the implementation of the boundary conditions.

8:45 AM *A4.2
NUMERICAL SIMULATION OF STRONG DISLOCATION-DISLOCATION INTERACTIONS. Klaus Schwarz, IBM Research, Yorktown Heights, NY.

Strong local interactions between individual dislocations have an important influence on phenomena ranging from the relaxation of heteroepitaxial semiconductor films to work hardening in metals. We have used our dislocation-dynamics simulation code (PARANOID) to study such interactions in a variety of circumstances. New results for blocking in strained-layer relaxation and for junction formation via forest interactions in metals will be presented.

9:15 AM A4.3
IN-SITU TEM DEFORMATION STUDIES OF DISLOCATION GENERATION AND MOTION IN HIGH-PURITY Mo SINGLE CRYSTALS. M. Jouiad, I.M. Robertson, University of Illinois, Dept. of Materials Science and Engineering; D.H. Lassila, LLNL, Livermore, CA.

The generation and motion of dislocations in high-purity single crystals of Mo have been observed in real time by deforming electron transparent specimens in-situ in a transmission electron microscope. At 300 K and at low levels of stress, a novel dislocation source was observed that generated a long, straight screw dislocation. The source was a dislocation tangle that existed in the annealed material. An edge dislocation emerged from the dislocation tangle and trailed behind it the screw dislocation. These screw dislocations were immobile at this low stress level. At higher stresses, the same dislocation tangle generated copious numbers of dislocations, but now by a pole mechanism. The nature of these tangles and the source operation mechanisms will be described. Screw dislocations in the matrix were now mobile, and they moved by nucleating large steps that spread rapidly along the length of the dislocation. These room temperature observations of dislocation generation and motion will be compared with results from current simulations in high-purity BCC materials, and with results from in-situ TEM deformation studies performed at lower temperatures.

9:30 AM A4.4
DISLOCATION DYNAMICS OF PLASTIC DEFORMATION IN MOLYBDENUM. Moono Rhee, Vasily Bulatov and Tomas Diaz de la Rubia, Lawrence Livermore National Laboratory, Livermore CA.

Early stages of plastic deformation and the underlying dislocation behavior in Mo are examined using our off-lattice DD algorithm. Initial dislocation arrangements were generated to mimick realistic TEM dislocation microstructures in the annealed Mo single crystals. The simulated deformation response indicates the onset of plastic yield and the development of characteristic cross-grid patterns dominated by the long screw dislocations. Although the initial microstructure has no dislocation sources, multiplication occurs naturally at the pinning points formed by non-coplanar superjogs moving towards each other along the screw dislocations. We present a detailed statistical analysis of the developing dislocation microstructures revealing their contribution to the observed yield behavior.

10:15 AM *A4.5
ATOMIC LEVEL SIMULATIONS OF DISLOCATIONS AND OF ELEMENTARY PROCESSES OF HARDENING IN FCC METALS. David E. Rodney, G. Martin, SRMP-CEA/Saclay, Gif-Sur-Yvette, FRANCE; M. Fivel, GPM2-INPG, Grenoble, FRANCE; V. Shenoy, R. Phillips, Div. of Engineering, Brown Univ., RI.

We present Molecular Dynamics and Quasicontinuum simulations of the interactions between a dislocation and two types of crystalline defects: (1) other dislocations, leading to junction formation and (2) irradiation induced glissile interstitial clusters. In both cases,we study the atomic level processes that occur during the simulations and compare them to TEM observations. We extract information from the simulations to be used in conjunction with higher level simulation methods. In particular, we show how new insights may be gained with respect to what governs the structure and strength of dislocation junctions by comparing our atomistic results with Dislocation Dynamics simulations. We also show how parameters evaluated at the atomic scale may be incorporated in Dislocation Dynamics codes to simulate irradiation hardening at the micron scale.

10:45 AM A4.6
DISLOCATION FOREST INTERACTIONS: SIMULATION AND PREDICTION. L.K. Wickham[1,2], K.W. Schwarz[2], J.S. Stolken[1]. [1]Lawrence Livermore National Laboratory, Livermore, CA; [2]IBM T.J. Watson Research Center, Yorktown Heights, NY.

Using linear elastic dislocation dynamics simulations, we show that junction formation between dislocations from various interacting slip systems can be predicted by a simple self–energy calculation. We find that this prediction is robust: anisotropic mobilities, dislocation curvature, and external stress produce little change in the simulation results for junction formation. The key to this success seems to be a separation of timescales, where movement of the far away dislocation arms (under, for example, external stress) is slow compared to the process of making a junction. The self-energy arguments give a rule for dislocation encounters which should allow a considerable saving in computational effort, allowing one to impose correct interaction outcomes without calculating the interactions in detail. We also find that dislocations often come together under attraction without forming a junction. The resulting "cross–linked" state provides an additional type of connection between dislocations. We present results on the persistence of junctions and cross–linked states under stress. (This work is performed under the auspices of U.S. Department of Energy and Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.)

11:00 AM A4.7
MODELING FOREST HARDENING AND DISLOCATION PATTERNING WITH A 2-D SIMULATION. D. Gomez-Garcia, B. Devincre and L. Kubin, LEM, CNRS-ONERA, Chatillon Cedex, FRANCE.

Based on the results of 3-D simulations of dislocation dynamics in pure fcc metals, a simplified 2-D model for multislip has been designed. This computer model quantitatively accounts for many dislocation properties like source multiplication, sessile junctions and cross-slip. Special attention was paid to the question of the dislocation fluxes at the boundaries of the simulation box. The results are found to correctly reproduce a linear increase of the flow stress with the square root of the dislocation density within 5 decades of density. The properties of the dislocation cell microstructure formed during deformation are discussed in relation with strain hardening properties.

11:15 AM *A4.8
DISLOCATION MOBILITY: FROM ATOMISTIC THEORY TO EXPERIMENTS. Vasily V. Bulatov, Lawrence Livermore National Laboratory, Livermore, CA.

Dislocation motion is known to control crystal plasticity under stress. Naturally, the mechanisms of dislocation mobility commanded much attention in the past and remain one of the key issues of materials physics at present. Although much is known about various generic factors affecting dislocation motion, quantitative description of dislocation mobility remains a challenge. We aim to develop a

computational theoretical framework for parameter-free prediction of dislocation mobility by kink mechanisms. Our approach combines atomistic calculations for the energetics of kink nucleation and migration with kinetic Monte Carlo simulations of dislocation motion under stress. So far, the results obtained for diamond cubic (Si) and bcc (Mo and Ta) materials generally agree with the experiments. In addition, several new behaviors for dislocation mobility are predicted and offered for experimental verification. This work is performed under the auspices of U.S. Department of Energy and Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

SESSION A5: DISLOCATION CORE PROPERTIES AND EFFECTS
Chairs: Vasily V. Bulatov and Rob Phillips
Wednesday Afternoon, December 1, 1999
Room 208 (H)

1:30 PM *A5.1
DISLOCATION CORE STRUCTURES AND DEFORMATION BEHAVIOR OF INTERMETALLIC COMPOUNDS. Michael J. Mills, The Ohio State University, Department of Materials Science and Engineering, Columbus, OH.

Ordered intermetallic compounds are of considerable technological and scientific interest due to their potential as structural materials for high temperature applications. In many cases, the attractive strength at high temperatures and unique flow properties of intermetallics are linked directly to their complex crystal structures (as compared with simple metals) which affect both the core structure and dissociation of dislocations. This presentation will focus on recent developments in our understanding of plastic flow in several ordered intermetallics, emphasizing the connection between the fine structure of dislocations and macroscopic mechanical properties. The results of experimental investigations using both high resolution and weak-beam TEM techniques will be described, as will the direct comparison of these fine structures with atomistic and continuum modeling approaches. The insight that these comparisons provide with respect to the unique flow properties in these alloys will also be discussed. Specific examples to be discussed include the anomalous flow strength behavior observed in Ni_3Al, the anisotropic flow properties of NiAl and the deformation of gamma-TiAl at higher temperatures.

2:00 PM A5.2
PROPERTIES OF THE DEFORMATION MICROSTRUCTURE IN Al-RICH GAMMA TiAl DEFORMED BY ORDINARY DISLOCATIONS. Fabienne Gregori, LPMTM, Universite Paris-Nord, Villetaneuse, FRANCE, Patrick Veyssiere, LEM, CNRS-ONERA, Chatillon, FRANCE.

In the near vicinty of the $< 021 >$ orientation, gamma-TiAl deforms via ordinary $1/2< 110 >$ dislocations. As for deformation by $< 011 >$ dislocations, the flow stress shows a peak at about 600°C. We present the result of an extensive microstructural investigation aimed at identifying the origin of this mechanical anomaly. The analysis was conducted in single crystals oriented for single slip. It is observed that ordinary dislocations tend to align themselves along the screw direction. Dislocation segmentation becomes gradually more pronounced with increasing deformation temperature. This effect is accompanied by a strong tendency towards cusp fomation. It is found that the immobilization along the screw direction takes place prior to dislocation pinning. In addition, dislocation show specific organization properties forming tight bundles at the peak temperature. The origin of the flow stress anomaly is discussed in relation with the appearance of a superstructure of the gamma phase.

2:15 PM A5.3
COMBINED CONTINUUM AND ATOMISTIC MODELING FOR THE PREDICTION OF ANOMALOUS YIELD STRENGTH. A.T. Paxton, Department of Pure and Applied Physics, Queen's University, Belfast, NORTHERN IRELAND; and Y.Q. Sun, Department of Materials Science and Engineering, University of Illinois, Urbana, IL.

The anomalous yield stress in intermetallic alloys with the $L1_2$ structure is predicted with the multiscale approach. On the mesoscopic scale, the long-range interaction between partial dislocations is formulated with anisotropic elasticity theory. On the atomistic scale, first-principle FLAPW method is used to calculate the surface energy of stacking faults coupling the partial dislocations. Results from both approaches are combined to predict and verify the transition of dislocation cores involving cross slip. The cross-slip behavior is in turn correlated with the anomalous yield strength. The theory is compared with experimental measurements of normal and anomalous materials.

2:30 PM A5.4
STUDY OF THE MECHANICAL BEHAVIOR OF BCC TRANSITION METALS USING BOND-ORDER POTENTIALS. M. Mrovec, V. Vitek, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA; D. Nguyen-Manh, D.G. Pettifor, Department of Materials, University of Oxford, Oxford, UNITED KINGDOM; M. Sob, Institute of Physics of Materials, Academy of Sciences of the Czech Republic, CZECH REPUBLIC.

Mechanical properties of the 4d (Nb and Ta) and 5d (Mo and W) transition metals are studied by computer simulation using the recently constructed bond-order potentials (BOP). These potentials are based on the real-space parametrized tight-binding method and the energy consists of the bond part that comprises contributions of d electrons, the central-force many-body part that reflects the environmental dependence of overlap repulsion arising from the valence sp electrons and a repulsive pair-wise contribution; the calculations scale linearly with the system size. In order to examine the accuracy and transferability of the potentials we have first evaluated the energy differences of alternate structures, investigated several deformation paths and evaluated the vacancy formation energies. These calculations are compared with the results of ab initio calculations and experiments. The calculations of the γ-surfaces, core structures of screw dislocations and structures of grain boundaries have been performed and compared with analogous studies made using the Finnis-Sinclair central-force many-body potentials. This comparison enables us to assess the importance of directional bonding in studies of mechanical behavior of the 4d and 5d transition metals. This research was supported in part by the Advanced Strategic Computing Initiative of the U.S. Department of Energy through LLNL, grant no. B331542 (MM and VV).

3:00 PM *A5.5
TRANSITION TEMPERATURES IN PLASTIC YIELDING AND FRACTURE OF SEMICONDUCTORS. P. Pirouz, Case Western Reserve University, Department of Materials Science and Engineering, Cleveland, OH.

Recent experiments on deformation of semiconductors show an abrupt change in the variation of the critical resolved shear stress, tY, with temperature, T. This implies a change in the deformation mechanism at a critical temperature Tc. In the cases examined so far in our laboratory and elsewhere, this critical temperature appears to coincide with the brittle-ductile transition temperature, TBDT. In this talk, the deformation experiments performed on the wide bandgap semiconductor, SiC, over a range of temperatures and strain rates will be described together with the characterization of induced dislocations below and above Tc by transmission electron microscopy (TEM). Based on the results, and those of Suzuki and coworkers in Tokyo on other compounds, some understanding of the different mechanisms operating at low and high temperatures in semiconductors has been obtained, and a new model for the brittle-ductile transition in these materials has been proposed.

3:30 PM A5.6
ATOMIC SCALE SIMULATIONS OF SCREW DISLOCATION CROSS SLIP IN Cu. T. Vegge[1,2], O.B. Pedersen[2], T. Leffers[2], and K.W. Jacobsen[1]; [1]Center for Atomic-Scale Materials Physics (CAMP) and Dept of Physics, Technical Univ of Denmark, Lyngby, DENMARK. [2]Risø Nat Lab, Roskilde, DENMARK.

Cross slip of screw dislocations is a fundamental process in plastic deformation, where it is involved both in the multiplication and annihilation of dislocations. The phenomena of cyclic saturation in fatigue and the onset of stage III in tensile deformation are thus generally believed to reflect the annihilation of screw dislocation dipoles activated by cross slip. It has recently become possible to address cross slip by purely atomistic simulations, thereby avoiding the problems associated with the structure and energetics of overlapping dislocation cores in elasticity theory. Atomistic simulations of non stress assisted cross slip of isolated, perfect screw dislocations, annihilation of screw dislocation dipoles, direct MD simulations of dipole annihilation rates, and cross slip of pre-constricted screw dislocations have been performed, using an effective medium theory (EMT) many body potential. We apply the nudged elastic band method to determine the minimum energy path for the cross slip process and we determine the cross slip activation energies of various configurations of screw dislocations with jogs and kinks. We also determine an attempt frequency for the dipole annihilation process based on direct MD simulations, this is done using harmonic transition state theory.

3:45 PM A5.7
EMBEDDED ATOM MODEL POTENTIAL–BASED DESCRIPTION OF THE ATOMIC STRUCTURE OF A DISSOCIATED EDGE DISLOCATION IN COPPER. L. Perondi*, M. Robles and K.

Kaski, Helsinki University of Technology, Laboratory of Computational Engineering, Espoo, FINLAND; *Permanent address: Instituto Nacional de Pesquisas Espaciais INPE, SP, BRAZIL.

The atomic structure of a dissociated edge dislocation in copper as a function of temperature is studied. Special attention is given to the core structure of the Shockley partials and the fault ribbon. The studies are carried out through Molecular Dynamics simulations. The atomic interactions have been modelled through an Embedded Atom Model (EAM) potential, the implementation of which has been specially designed for this study. The temperature effects have been implemented through a Nosé-Hoover thermostat.

4:00 PM A5.8
ATOMISTIC SIMULATION OF TRANSONIC DISLOCATIONS. Jonathan A. Zimmerman and Huajian Gao, Division of Mechanics and Computation, Stanford University, Stanford, CA; Farid F. Abraham, IBM Almaden Research Center, San Jose, CA.

Recent work has been done on the analysis of elastic stress singularities, such as cracks and dislocations, which propagate at supersonic speeds. This work has been motivated by experiments in high-speed impact and the mechanics of tectonic faults. Gumbsch and Gao have performed atomistic simulations where, given sufficient loading, dislocations are created and travel at transonic velocities (speeds which are greater than the material's shear wave speeds but less than the longitudinal wave speed). These simulations show dislocations in isotropic BCC tungsten which travel transonically at a speed $\sim 1.4\, c_{shear}$, a value corresponding to the radiation-free (r-f) state for glide motion. Also shown is the existence of a forbidden zone of velocities: defects are *created* with supersonic velocities and cannot be accelerated from subsonic speeds into the transonic regime. Using continuum elasticity, Gao, Huang et al. derived expressions for the r-f velocity of shear cracks and dislocations, shown to be the same for the two defects, for propagation in both isotropic and anisotropic media. We have performed atomistic simulations showing dislocation nucleation at crystal surface ledges, believed to occur in cases such as heteroepitaxial thin films on substrates. Molecular dynamics simulations show dislocations nucleated at either super- or subsonic velocities, depending upon the ambient temperature, and accelerated to speeds close to the radiation-free speed. While this acceleration contradicts existing theories, an explanation can be made from type of dislocations emitted. This paper reviews the Stroh-type analysis that calculates the theoretical r-f speed for our particular crystal geometry, and compares it to measurements of the speed of the dislocations nucleated in these simulations. Our findings are particularly exciting considering these simulations were not specifically engineered for the purpose of creating transonic defects, but show agreement with anisotropic elasticity theory nonetheless.

4:15 PM A5.9
MODELING INDENTATION USING THE LOCAL QUASI-CONTINUUM FORMULATION. Greg S. Smith, Umesh V. Waghmare, Efthimios Kaxiras, Harvard University, Div of Engineering and Applied Sciences, Cambridge, MA; Ellad B. Tadmor, Technion–Israel Inst of Technology, Faculty of Mechanical Engineering, ISRAEL.

Indentation experiments have proven very useful in probing the mechanical and high pressure behavior of a variety of materials. An indented system is very complicated, with anisotropic nonlinear elastic effects and plastic deformation occurring near the indenter. This complexity makes it difficult to understand how microscopic processes affect macroscopic response, but in certain cases computer simulations could help elucidate the relationship. Unfortunately, computer simulations of indented systems are very challenging, since even in nanoindentation experiments the indenter tip radius (on the order of 1000 angstroms) and sample size are much larger than the atomic scale, while the large compressions and shears in the system require an accurate description of atomic configurations very far from equilibrium. The local quasicontinuum method, extended to handle complex Bravais lattices, [1] is well-suited for this type of problem. By embedding an atomistic potential in a finite element framework, the formulation maintains the computational efficiency of the finite element method, but naturally incorporates crystalline anisotropy, nonlinear elastic effects, and the possible occurrence of structural phase transformations. We apply this method to model three-dimensional indentation of silicon and lead titanate, $PbTiO_3$. For silicon, the Stillinger-Weber empirical potential is used. With the aid of a simple model, we are able to make direct comparisons between simulated and experimental load vs. electrical resistance curves. For $PbTiO_3$, we use an energy functional whose parameters are determined via density functional calculations. We explore hysteretic effects in the load vs. displacement curve, and polarization patterns that form in the course of indentation.

[1] E.B. Tadmor, G.S. Smith, N. Bernstein, and E. Kaxiras, Phys. Rev. B **59**, 235 (1999).

4:30 PM *A5.10
DIFFERENT RELAXATION MODES OF EPITAXIAL AuNi ALLOYS. Jany Thibault, Cyril Dressler, Pascale Bayle-Guillemaud, CEA/DRFMC/SP2M, Grenoble, FRANCE.

It will be shown that the mechanism that takes place at a nano-scale level to release the internal stresses in materials might be more complex than the expected one which involves only individual dislocations. This will be illustrated on a $Au_{1-x}Ni_x$ alloys which is representative of alloys with a large size effect and with a large miscibility gap. The structure and the stability of $Au_{1-x}Ni_x$ alloys grown at room temperature by MBE on (001) Au buffer has been investigated by high resolution electron microscopy as a function of the alloy thickness and as a function of heat treatments. In fact the expected dislocation mechanism occurs only for low misfit alloys i.e alloys with a low Ni concentration. At higher Ni concentrations the dislocation mechanism might be biased and other mechanisms take place. Furthermore different mechanisms can successively take place. Mixing at the interface, twinning, phase transformation have been seen to release the stress. The evolution of the $Au_{1-x}Ni_x$ alloys with temperature has been also investigated by HREM and it will be shown that despite the phase diagram, which predicts a phase separation, an ordering occurs in the alloy driven by the stress. In-situ HREM allows to study the very early stages of phase separation. In fact the occurrence of the ordered AuNi phase fully relaxes the stress. It is noticeable that atomistic simulations made independently from this work predict the same behaviour. The alloy evolution has been followed also by in-situ X-rays diffraction, which allows numerous specimens and various conditions to be explored.

SESSION A6: POSTER SESSION:
DISLOCATION DYNAMICS
Chairs: Lyle E. Levine and Michael J. Mills
Wednesday Evening, December 1, 1999
8:00 P.M.
Exhibition Hall D (H)

A6.1
A TEM STUDY ON THE DYNAMIC PROPERTIES OF DISLOCATIONS IN BCC METALS. Luke M. Hsiung, Lawrence Livermore National Laboratory, Materials Science and Technology Division, Livermore, CA.

To support dislocation dynamics simulation and theoretical modeling of BCC crystal plasticity, dislocation substructures of high-purity Ta and Mo crystals have been examined and studied using transmission electron microscopy (TEM) techniques. For the success of dislocation dynamics simulation, it is of importance to pursue a systematic study on the dynamic properties of dislocations including dislocation multiplication, motion, and interaction. Since initial dislocation structures (dislocation density, configuration, free dislocation link, kink and jog on dislocation line...) can affect all the aspects of dislocation properties during plastic deformation, the as-annealed dislocation structures as well as the dislocation structures after quasi-static compression and shock deformation are studied and compared. Emphasis is placed on the dislocation multiplication and the dynamic motion of dislocations. The formation of cross-grid screw dislocation, dislocation junction, dislocation dipole and shock-induced shear transformations in BCC metals are critically reviewed and discussed.

A6.2
AB INITIO STUDY OF DISLOCATIONS IN MOLECULAR CRYSTALS. Maija M. Kuklja, A. Barry Kunz, Electrical Engineering Department, Michigan Technological University, Houghton, MI.

Dislocations are known to arise in solids during crystal growth and due to different external effects such as heat, shock, impact, pressure, etc. Experimentally, dislocations in crystalline cyclotrimethylene trinitramine (aslo known as RDX) have been studied by several researchers. The electronic structure of molecular crystals with edge dislocations was not studied so far. An ab initio study of the electronic structure of the solid explosive RDX crystal containing the [001] edge dislocations was performed by means of the Hartree-Fock periodic method combined with the many-body perturbation theory. Additionally, we have studied how strong compression (for example, shock/impact wave) affects the RDX crystal with edge dislocations. We found that an external pressure causes a significant decrease of the optical gap for both the perfect material and the crystal with dislocations. The edge dislocations produce local electronic states in the optical gap whereas the external pressure moves these states deep within the band gap. This contributes strongly to properties of the RDX crystals creating favorable conditions for the N-NO2 chemical bond rupture due to exciton formation. Relations between the edge

dislocations, hot spots formation, and the sensitivity of RDX to detonation are discussed in detail. A new mechanism of detonation initiation is proposed. As an illustration of complexity of the present calculations one can mention the unit cell of the defective crystal consists of 210 atoms, and this unit cell possesses a total 1140 electrons, of which only 300 are core electrons. A split valence basis set as used here consists of 1470 atomic functions. A single HF calculation with CRYSTAL95 on Multiprocessor SUN Enterprise 4000 system with 12 Ultra Sparc II processors (250MHz) in a parallel version with four processors runs for 2 days demanding significant resources of the disk memory. The essential conclusion is that edge dislocations in the RDX crystal could serve as hot spots, which are characterized by a local internal stress and by a reduced optical gap. The impact wave propagating through the crystal stimulates a further dramatic gap reduction increasing the probability of electron excitation. This, in turn causes molecular dissociation via an excitonic mechanism and start a chain reaction and explosion.

A6.3
SIMULATION OF DISLOCATION DYNAMICS IN Ni_3Al: A STUDY OF VELOCITY AUTOCORRELATIONS. C.K. Erdonmez, D.C. Chrzan, University of California, Dept of Material Science & Mineral Engineering, Berkeley, CA.

This work continues earlier efforts to understand the yield stress anomaly in $L1_2$ alloys using computer simulations of dislocation motion. The elastic self-interaction of dislocations are taken into account within an isotropic approximation and simple rules are used to account for the cross-slip process in the 2D geometry of the simulation. The velocities of single dislocations are studied for a choice of parameters appropriate for the yield strength anomaly in Ni_3Al. It is found that dislocation velocities are a non-linear function of stress. At typical temperatures, dislocations self-immobilize rapidly at low stress and move with little hindrance at high stresses. Above the threshold stress required to move single dislocations, fluctuations in dislocation velocity are seen to persist for longer times at lower stresses. The velocity-fluctuation auto-correlation function is studied as a function of stress. The characteristic decay time of the correlations increases rapidly as one approaches the threshold stress for dislocation mobility from above. This rapid increase can be used to identify the threshold stress as a function of physical parameters.

A6.4
MODELING COLLECTIVE DISLOCATION DYNAMICS IN ICE SINGLE CRYSTALS. M.-Carmen Miguel, A. Vespignani, The Abdus Salam International Centre for Theoretical Physics, Trieste, ITALY; S. Zapperi, PMMH-ESPCI, Paris, FRANCE.

The viscoplastic deformation of crystalline materials such as ice single crystals, involves the motion of a large number of dislocations. Although the dynamics of an individual dislocation is a fairly well characterized phenomenon, the collective behavior of a large number of these defects appears to be an amazingly rich but poorly understood problem. As a result of their interactions, dislocations tend to move cooperatively giving rise to a rather complex and heterogeneous slip process. The complex character of the collective dislocation dynamics reveals itself in experiments of acoustic emission (AE) [1]. Sudden local changes of inelastic strain generate AE waves. The AE signals detected seem to correspond to the synchronous motion of several dislocations, likely to occur for example during the breakaway of a pile of these defects. The AE experiments, however, have only access to information resulting from the interplay of various magnitudes. Thus, the physical interpretation of the generated AE waves remains a major difficulty. We propose a model to study the plasticity of ice single crystals which starts with the simulation of the system in rather general and realistic conditions. The model includes the long-range character of the interaction among dislocations, as well as the possibility of mutual annihilation of these line defects characterized by its Burgers vector. With our approach we are able to probe the dislocation patterns, which result from the dislocation dynamics. Furthermore, our results exhibit features characteristic of driven dynamic critical phenomena such as scaling behavior, avalanche dynamics, and singular response functions. Some of these results account for the experimental findings reported for single crystals of ice under creep deformation, like the power-law distributions of the AE amplitudes observed sistematically in experiments [1].
[1] J. Weiss and J.R. Grasso, J. Phys. Chem. B **101**, 6113 (1997).

A6.5
NUCLEATION, BLUNTING OR PROPAGATION OF A NANOCRACK IN DISLOCATION-FREE ZONES OF THIN CRYSTALS. Q.Z. Chen, W.Y. Chu, K.W. Gao, B. Gu and Y. Zhang, Department of Materials Physics, University of Science and Technology Beijing, Beijing, CHINA.

Nucleation, blunting and propagation of nanocracks in dislocation-free zone (DFZ) ahead of crack tips in ductile and brittle metals have been investigated by tensioning *in situ* with a TEM, and analysed using microfracture mechanics. The results show that in either ductile or brittle metals, many dislocations could be emitted from a loaded crack tip and a DFZ formed after equilibrium. The stress in the DFZ may be up to the cohesive strength of the material, and then a nanocrack is initiated in the DFZ or directly from the crack tip. In ductile metals, the nanocrack is blunted into a void or notch during constant displacement. In brittle metals, the nanocrack propagated as a cleavage microcrack rather than being blunted.

A6.6
THE ENERGETICS OF DISLOCATION-OBSTACLE INTERACTIONS BY 3-D QUASICONTINUUM SIMULATIONS. Kedar Hardikar and Rob Phillips, Div. of Engineering, Brown Univ., Providence, RI.

A recently developed method to incorporate periodic boundary conditions in three dimensional quasicontinuum simulations is used in study of interactions between dislocation and localized obstacles to glide. The objective of this work is to obtain the energy of interaction for various configurations as a dislocation infinite in extent overcomes an array of obstacles such as point defects, precipitates and other dislocations, under the action of external applied stress. The results are presented in the form of energy of interaction as a function of the reaction coordinate and are used to characterize the strength of various interactions. These results are then used to develop models which can be used as a basis for analysis of the many body problem in which a dislocation interacts with many such defects.

A6.7
Al-RICH GAMMA-TiAl SINGLE CRYSTALS DEFORMED BY <011] DISLOCATIONS OVER THE DOMAIN OF FLOW STRESS ANOMALY. Fabienne Gregori, LPMTM, Universite Paris-Nord, Villetaneuse, FRANCE; Patrick Veyssiere, LEM, CNRS-ONERA, Chatillon, FRANCE.

Al-rich gamma-TiAl single crystals deform essentially by motion of <011] dislocations and show a peak of flow stress located between about 700°C and 950°C, depending on load orientation (Inui et al., Phil Mag. A, 75 (1998) 395). We present mechanical data of such alloys oriented so as to deform by single slip. These data are complemented by TEM observations in samples strained at room temperature, 400°C, 600°C and 800°C. Our study addresses (i) the properties of dislocation organization, (ii) the dissociation mode of <011] dislocations in their slip plane, (iii) the locking properties of <011] dislocations and (iv) the conditions of formation of stacking fault dipoles. These findings are discussed in the light of results available in the literature.

A6.8
ENERGY LOSS FROM A BIASED ISOLATED FRANK-READ SOURCE UNDER AN OSCILLATORY DRIVING STRESS. P. Alex Greaney and D.C. Chrzan, Dept. of Materials Science and Mineral Engineering, University of California, Berkeley, CA and Division of Materials Science; Ernest Orlando, Lawrence Berkeley National Laboratory, Berkeley, CA.

The dissipative losses contributing to acoustic attenuation from a single Frank-Read source are studied. A computer model of a dislocation in an isotropic linear elastic continuum is used to model an isolated, cyclicly driven, Frank-Read source. The dislocation is treated as massless and is assumed to obey a linear drag law. The stress on the dislocation is the sum of a static biasing stress, a sinusoidal driving stress and the dislocation self stress. Energy losses are calculated for driving angular frequencies in the range from 10 kHz to 5 MHz. The operating stress of the Frank-Read source increases with driving frequency. The dislocation behaves like a linear oscillator at low stresses and high frequencies, but produces large energy losses near the critical configuration of the dislocation source. A comparison is made with Granato-Lücke theory for unbiased sources, and with a simple circular dislocation approximation. This research is supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Science Division under Contract No. DE-AC03-76SF00098.

A6.9
COMPUTER SIMULATION OF THE EFFECT OF COPPER ON DEFECT PRODUCTION AND DAMAGE EVOLUTION IN FERRITIC STEELS. J. Manuel Perlado, Jaime Marian, Dario Lodi, DENIM, Universidad Politécnica de Madrid, Madrid, SPAIN; Tomás Díaz de la Rubia, LLNL, Chemistry and Materials Division, Livermore, CA.

It has long been noticed that the effect of Cu solute atoms is important for the microstructural evolution of ferritic pressure vessel steels under neutron irradiation conditions. Despite the low concentration of Cu in steel, Cu precipitates form inside the α-Fe surrounding matrix and considerably contribute to the hardening of

the material through dislocation interactions. The neutron damage associated to these particular conditions and the formation and evolution of the precipitates have not yet been completely understood. Also, the processes and effects related to these mechanisms are not directly observable by any experimental means so a computer simulation methodology based on Molecular Dynamics and Kinetic MonteCarlo has been used to approach the study of a Fe-Cu alloy. The study has been made using the MDCASK code in which the Ackland (Finnis-Sinclair) many-body potential has been implemented. At DENIM, we have carried out many high-energy displacement cascades for energies ranging from 1 to 20 keV to assess the effect of the Cu concentration on the microstructural evolution of the alloy. Also, formation, binding and migration energies corresponding to diverse Fe-Cu defect structures have been calculated. Values of 0.6 eV and 6.2 eV have been recorded for the Cu vacancy formation energy in a Fe-Cu solution and for the Fe-Cu dumbbell formation energy. Cu solute atoms exhibit a natural tendency to attract defect structures while Cu interstitials seem to be less mobile than Fe interstitials in the same conditions. Finally, a preliminary Cu precipitation tendency has been observed in our KMC simulations.

A6.10
OPTIMIZED SIMULATION OF DISLOCATION DYNAMICS: METHOD AND VALIDATION TESTS. R. Madec, B. Devincre and L. Kubin, Laboratoire d'Etudes des Microstructures, CNRS/ONERA, Chatillon, FRANCE.

During the 90s, the principles of a 3-D simulation of dislocation dynamics at a mesoscopic scale have been developed. Such simulation combines a simplified description of the core properties with the more rigorous elastic theory of dislocations to understand the formation and the dynamics of dislocation microstructures. Calculations with this model were first done for pure single crystals, at small strains and with simple boundary value problems. More recently, the simulation has been successfully combined with a finite element code to study samples with complex boundary conditions. Nevertheless, persisting limits to the computer model are existing. First, its CPU requirement increases extremely fast with increasing number of segments. Hence, computations are restricted to small samples ($\approx 3500\mu m^3$) and small plastic strains ($\approx 1\%$). Secondly, the simplicity of the edge-screw line model used to discretize dislocation curvature makes the calculation of the elastic properties at short distances difficult. For these reasons, a new computer model was designed. Initially, only two possible directions for the dislocation segments were considered for each slip system: one lying in the screw direction and the other one in the edge direction. Now, additional mixte segments are accounted for in each slip system. It is shown that this discretization procedure substantially reduces the segment number per unit length, as well as it produces a better description of the self stress field of dislocations at short distances. In the present report, results of the validation tests made with our new model are shown and critically discussed by comparison with other existing models.

A6.11
TEM ANALYSIS OF PARTIAL DISCLINATION CONFIGURATIONS IN COLD-ROLLED COPPER. V. Klemm, M. Seefeldt and P. Klimanek, Freiberg Univ of Mining and Technology, Freiberg, GERMANY.

The rotational parts of the microstructure evaluation under plastic deformation of metallic materials up to large strains and the coupling between rotational microstructure elements and the macroscopic behavior can be modelled with the help of the disclination concept. TEM microdiffraction experiments are used for local misorientation measurements which allow the identification of the partial disclinations and of their configurations. Copper single- as well as polycrystals rolled down to 50 % and 70 % thickness reduction at room temperature were investigated and partial disclination dipoles were found in triple junctions due to splittings of dense disloaction walls (DDW) into first generation microbands (MB1). The detailed characterization of partial disclination dipoles includes the determination of misorientation matrices, of Frank vectors of the disclinations and of rotation vectors of the dislocation walls around the disclination lines. These parameters for mesoscopic structure elements provide an efficient tool for the comprehension of complex configurations of dislocations as microscopic structure elements.

A6.12
THE EFFECT OF INTERNAL STRESS ON THE FLOW STRESS. Shig Saimoto, Haio Jin, Ke Zhang, Peter Poruks, Dept. Materials & Metallurgical Engineering, Queen's University, Kingston, Ontario, CANADA.

In the phenomenon of plastic deformation, the precise role of the internal stress which inherently evolves with strain hardening is still not well understood and leads to ambiguities in the quantitative analysis of thermally activated flow. The composite work hardening theory of Mughrabi predicts that the internal stress in the tangled walls are opposite in sign to that in the cells. However, the flow stress is incapable of detecting either contribution. This means that the stored work measured by direct X-ray studies would not quantitatively correlate to the flow stress and the resulting recrystallized structure. Our recent studies on metal matrix of high purity formed by gettering specific solutes, results in a fine structure which manifests continuous/dynamic recrystallization with grain sizes less than 2 μm. The behaviour of the fractional residual stress parameter, which is a relative measure of the line broadening between $K_{\alpha 1}$ and $K_{\alpha 2}$, does not correlate to that of hardness with anneal recovery times. To ascertain that the residual stresses are indeed decreasing rapidly whereas the hardness is not, in situ lattice determinations were made using a specially constructed X-ray hot stage. These results show that in polycrystalline deformation the residual stresses arise due to strain compatibility among the grains, of the order of less than 0.0001, and decrease to zero only after discontinuous large grain growth. The flow stress is due to the dipole dislocation density in the tangles walls.

A6.13
MULTISCALE MODELING OF ELECTROMECHANICALLY-DRIVEN VOID DYNAMICS AND FAILURE IN METALLIC THIN-FILMS. M. Rauf Gungor and Dimitrios Maroudas, University of California, Santa Barbara, Department of Chemical Engineering, Santa Barbara, CA.

The failure of metallic thin films due to stress and electromigration-induced void propagation and morphological evolution is a major reliability problem in microelectronics. In this paper, we present a multiscale theoretical and computational study of electromechanically-driven failure of metallic thin films mediated by transgranular void dynamics aiming at quantitative predictions and comparisons with experimental measurements. Our analysis is based on linking self-consistent mesoscopic dynamical simulations of interface morphological evolution with atomistic calculations of interfacial properties and molecular-dynamics (MD) simulations of void evolution under stress. Our mesoscopic simulations are based on surface transport modeling under mechanical loading and surface electromigration. Galerkin boundary-element computations of the electric field and strain field distribution on the evolving void surface and the metallic film boundaries are coupled self-consistently with the propagation of the void surface and the rest of the domain boundary. The rich nonlinear dynamical behavior of transgranular voids over a wide range of electromechanical forcing is explored in a multi-dimensional parameter space; the corresponding parameters express the relative strengths of the external fields, the void size, and the anisotropy of atomic mobility on the void surfaces and of the applied stress tensor. A systematic parametric search is conducted to establish the range of morphological stability for transgranular voids. The general mode of thin-film failure under simultaneous action of electric fields and mechanical stresses consists of the coupling of two modes of morphological instability: the first is electromigration-driven and leads to wedge shape formation and faceted slit propagation, while the second is stress-driven and leads to formation of fine-scale crack-like features. More importantly, we demonstrate the possibility of failure inhibition through proper tailoring of processing conditions to achieve a given film texture and range of stress state and level in the films. Furthermore, we demonstrate that the range of void morphological stability depends strongly on the anisotropy of the applied stress, i.e., as the stress state changes from hydrostatic to uniaxial. The dynamics of the observed crack-like features on the void surface is investigated further based on large-scale MD simulations using an embedded-atom-method parametrization for Cu. Our MD results elucidate the role of dislocation-mediated mechanisms on void growth and shape change and are used for the incorporation of dislocation dynamics into our mesoscopic modeling framework.

A6.14
MECHANICAL LOSS ASSOCIATED WITH STRESS ANOMALY IN Ni_3Al AND Ni_3(Al,Ta) SINGLE CRYSTALS. E. Carreño-Morelli[1], B. Cheng[1], M. Demura[2], R. Schaller[1], N. Baluc[1] and J. Bonneville[1]; [1] Ecole Polytechnique Fèdèrale de Lausanne, Institut de Gènie Atomique, Lausanne, SWITZERLAND; [2]National Research Institute for Metals, Mechanical Properties Division, Tsukuba, JAPAN.

Dislocation dynamics in Ni_3Al and Ni_3 (Al,Ta) single crystals has been investigated by measuring mechanical loss and shear modulus as a function of temperature in the range 100 K - 1300 K. Measurements were performed in free and forced torsion pendula. The mechanical loss spectra are divided in two temperature domains separated by a relaxation peak at about 950 K (1 Hz). This relaxation peak has been attributed to the stress re-orientation of Al-Al elastic dipoles in the (111) octahedral plane. In the low temperature range, which corresponds to the anomaly domain of the flow stress, the mechanical loss of pre-deformed specimens is strongly dependent on measurement oscillation amplitude and predeformation strain. Pre-deformation (performed at room temperature or 100 K) is at the origin of a broad

maximum located near 300 K, which is observable only for measurement strain amplitudes higher than 10^{-4}. This maximum completely vanishes after heating up to 500 K. Thermal cycling experiments performed at temperatures below 500 K, have evidenced a progressive and irreversible decrease in mechanical loss which is more pronounced during coolings. This behaviour is discussed in terms of pinning of screw dislocation segments via cross-slip from the (111) onto the (010) planes (Kear-Wilsdorf locks). After exhaustion of mobile dislocation segments in the low temperature domain, a new plasticity appears at high temperature resulting in a mechanical loss exponential background, which may be attributed to the dislocation motion on the {001} cube planes.

A6.15
MESOSCOPIC ANALYSIS OF NEAR-SURFACE PLASTIC DEFORMATION INDUCED BY THERMOMECHANICAL FATIGUE ON 316L STAINLESS STEEL PART 1/2: EXPERIMENTS. Christian F. Robertson, S. Poissonnet, A. Fissolo, DTA, CEA Saclay, Gif sur Yvette, FRANCE.

Thermo-mechanical fatigue is an important life limiting factor for materials used in power plant cooling systems. Indeed, transgranular fatigue cracks induced by thermo-mechanical loadings with random temperature ranges up to 300K have recently been observed [1]. Surface effects like topography and stress fields due to sub-surface dislocation microstructures constitute possible causes for precocious fatigue crack nucleation [2]. The present study thus concentrates on the analysis of dislocation microstructures included within a small volume (typically $20 \times 20 \times 20 \mu$m), located close to the surface. This defines a mesoscopic scale for which transmission electron microscopy (TEM) observations can be directly compared to results from 3D numerical simulations of discrete dislocation dynamics [3].
The particular case of an indent induced plastic zone will be here selected, since this microstructure is well characterized and confined close to the indented surface [4]. Hence, the following experimental procedures have been undertaken. First, arrays of identical 50nm deep indents are performed on 3 millimeter 316L steel disk samples. Next, the samples are cyclically heated up and cooled down at a rate of 0.2 Hertz [5]. The total temperature variation is so selected as to keep the resulting strain amplitude within the elastic regime. After the cycling, thin foils are cut out of the disks using back side electro-polishing technique [4]. A comprehensive analysis of the TEM observations has been facilitated by detailed results from numerical simulations of the performed tests (see part 2/2).
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A6.16
MESOSCOPIC ANALYSIS OF NEAR-SURFACE PLASTIC DEFORMATION INDUCED BY THERMOMECHANICAL FATIGUE ON 316L STAINLESS STEEL PART 2/2: SIMULATIONS. Marc C. Fivel, GPM2/CNRS, Grenoble, FRANCE; Christian F. Robertson, DTA/SRMA, CEA Saclay, Gif sur Yvette, FRANCE.

3D discrete dislocation dynamics (DDD) simulations have proven to be a powerful tool to provide a comprehensive interpretation of the formation of dislocation microstructures [1]. It is here used to help understand the mechanisms involved in thermomechanical fatigue of 316L stainless steel.
First, a 3D indent induced dislocation microstructure is generated using the same method as described in [1]. The generated dislocation microstructure is then subjected to time dependent thermo-mechanical loading. The cyclic applied stress is superimposed on the internal stress field associated with the dislocation segments. The thermo-mechanic stress tensor is chosen to be homogeneous in the simulated box, the latter being small compared to the grain size. For each time step, an elastic boundary problem is solved using a finite element method. The cyclic loading is applied in a quasi static manner, which means that at each loading step, the segments move until they reach a stable configuration. The applied thermal load is then changed according to experimental measurements (see Part 1). After a given number of simulated cycles, the numerically generated dislocation microstructure is compared to the experimental one, obtained under the same conditions. Direct comparisons with TEM micrographs are performed on the resulting dislocation microstructure for several diffracting vectors $\mathbf{g}$.
M.C. Fivel, C.F. Robertson, G.R. Canova and L. Boulanger, Acta Mater., **46**(17), pp. 6183-6194, 1998.

A6.17
SIMULATION OF EQUILIBRIUM DISTRIBUTION OF DISLOCATION STRUCTURES IN bcc SINGLE CRYSTALS UNDER CYCLIC LOADING. S.B. Biner and J.R. Morris, Ames Laboratory, Iowa State University, Ames, IA.

We are investigating the collective motion of large number of discrete edge dislocations in bcc single crystals under cyclic loading using a numerical method that combines the finite element method and multi-pole expansion algorithm. The dislocations are modeled as line defects in a linear elastic medium. At each instant, superposition is used to represent the solution in terms of the infinite-medium solution for the discrete dislocations and a complementary solution that enforces the boundary conditions. Annihilation of dislocations, generation of new ones and dislocation pinning at obstacles are simulated through a set of constitutive models. The evolution of Bauschinger-effect, hardening and softening behavior is correlated with the cyclic load levels and the parameters of the constitutive model for the collective behavior of dislocations. We will briefly discuss the details of the parallel implementation of the numerical method.

A6.18
THE INFLUENCE OF STRAIN-RATE ON COOPERATIVE DISLOCATION GENERATION IN CRYSTALS: APPLICATIONS TO THE BRITTLE-DUCTILE TRANSITION. M. Khantha and V. Vitek, Dept of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA.

The mechanism of cooperative dislocation generation in loaded crystals can cause the formation and expansion of many dislocation loops without any energy barrier above a critical temperature [see Mat. Sci & Eng. A234-236, 629 (1997)]. Below this temperature, an activation barrier for the formation and expansion of dislocation loops exists but it decreases progressively as the temperature increases. This is unlike the activation barrier for the expansion of a single dislocation loop. At the present stage the model represents a static description of the instability without considering the possibility that thermally activated generation and glide of dislocations can occur below the critical temperature. In this paper, we discuss how the macroscopic glide of dislocations below the critical temperature can influence the onset of the cooperative instability. We present a model for the dependence of the critical temperature on the rate of loading and examine its relevance to the strain-rate dependence of the brittle-ductile transition.
This research was supported by U.S. Air Force Office of Scientific Research grant F49620-98-1-0245.

A6.19
STUDY OF ELECTRICAL PROPERTIES OF DISLOCATIONS IN ZnSe AND ZnS USING ELECTRIC FORCE MICROSCOPY. Victor F. Petrenko, Guofeng Bai, Dartmouth College, Thayer School of Engineering, Hanover, NH.

Electric force microscopy (EFM) was used to determine an electric charge of different dislocation in ZnSe and ZnS and to measure the effect of these dislocations on conductivity and photoconductivity of these materials. Undoped single crystals of ZnSe and ZnS with sphalerite structure were used in this study. Dislocations were induced in the crystals by either macroscopic plastic deformation at constant strain rate, or by micro-indentation, or by scratching. We have studied the electric charge of individual dislocations and dislocation bands. In all cases only dislocations that emerge on {110} cleavage planes were studied. A type of dislocations (perfect, partial, perfect dissociated, screw, edge, 60-degree) was determined by measuring surface topography in intermittent mode of SFM [1]. Both cation-type (Zn) and anion-type dislocations was found and studied. Electrically charged dislocations emerging on the surface of a crystal generate electrostatic potential above the surface. This potential can be detected and measured with EFM. Comparison of the dislocation-induced potential with a theoretical model enabled us to estimate an electric charge of static dislocations in ZnSe and ZnS. In addition to these experiments we studied local changes that small groups of dislocations produced in electric conductivity and photoconductivity of ZnSe and ZnS. For that purpose we induced a DC current in the crystals and then performed scans of electric potential over the crystal surface. In a uniform semiconductor specimen the potential changes linearly with lateral coordinates. While new dislocations linear dependence is distorted due to the local change in electric conductivity. The shape and magnitude of the distortion provide information on the donor- or acceptor-type behavior of the dislocations. The experimental results on electric charge and acceptor-type effect were then compared with known theoretical models. 1. O. Yu. Nickolayev and V.F. Petrenko, Study of dislocations in ZnS and ZnSe by scanning force microscopy, 1994. J. Vac. Sci. and Technol., B,12 (4) p. 2443.

A6.20
DISLOCATION-IMPURITY INTERACTIONS IN II-VI

MATERIALS. Valery P. Kisel and Svetlana A. Erofeeva, Institute of Solid State Physics, RAS, Chernogolovka, Moscow, RUSSIA.

An asymmetry of the mobility of 60-degree alfa and screw dislocations in pure and impure InSb, GaAs single crystals has been studied as a function of shear stess, temperature, number of loadings and the duration of pauses between them (restore time). The observed synchronous decrease in the free path length, l, and the mean number of mobile dislocations, n, under periodic tensile-compressive and monotonic multiple tension or compressive loadings are most clearly manifested for dislocations prone to a noticeable cross-slip (screws containing beta-partials) or for the screws being exposed to the maximal value of applied stress in the direction perpendicular to the slip plane [1]. The duration of pauses (restore time) between the consequtive loadings, the form of the loading impulses (the loading and unloading stress rates), their time lengths (frequency of stress pulses) and the stress level play the key-role in hardening and softening of crystals under the load. The scaling of the stresses for dislocation fixed pathlengths (fixed number of mobile dislocaions) and dislocation multiplication stresses, fracture stresses under different stresses shows that every point of micro- or macrodeformation curve is closely interconnected with the other points up to macroscopic fracture and damage due to the same micromechanisms, and the values of deformation stress are governed by sample prehistory and the scale length of observation: high differences in density of matrix defects and impurity nanoprecipitates, grain boundaries at various dislocation pathlength scales may infringe the universality of the above scaling law. All the data and the numerous published results on microscopic and macroscopic can be unambiguously explained using a universal model of dislocation motion and multiplication due to conservative or non-conservative motion of jogs, kinks, dislocation bowing and climb. [1] Kisel, V.P. et al., Phil. Mag., 67A, 343 (1993).

A6.21
EVALUATION OF THE CONSTANT LINE TENSION APPROXIMATION IN AN ATOMISTIC CONTEXT.
David L. Olmsted, Rob Phillips, Brown Univ, Div of Engineering, Providence, RI.

In practice, much of the work using dislocations to investigate or explain metallurgical phenomena such as precipitate hardening, dislocation sources, etc., is based on the constant line tension approximation of J. Friedel. We examine this approximation in multiple contexts, including, in particular, an atomistic context. The strategy adopted in this work is to carry out a series of calculations of the structure and energetics of dislocation lines for a number of different line orientations. The resulting energies are compared with those expected on the basis of models from linear elasticity. In addition, we consider the atomic-level structure of such dislocations when they bow out in the presence of an applied stress.

A6.22
INVESTIGATION OF DEFECT STRUCTURES IN PLASTICALLY DEFORMED STAINLESS STEEL 10X18H10T BY POSITRON ANNIHILATION METHOD. Adham A. Paiziev, Asad M. Karimov, Institute of Electronics, Dept. of Positron Diagnostics, Tashkent, UZBEKISTAN.

The modern methods of the microstructure control most be used to predict the strength characteristics of the construction materials and industrial goods. In this connection, we present the experimental results on the electron-positron annihilation (EPA) data for plasically deformed stainless steels samples 10X18H10T and compared with AISI 316 (Fe 65.3%, Cr 18.1%, Ni 12.2%, Mn 1.5%, Mo 1.4%, Si 1.2%, Co 0.3% /1/). The angular distributions of annihilation photons (ADAF) of a stainless steel specimens in an interval of a strain from 2 up to 20% are measured. Is shown, that the half-width of a ADAF curve monotonically decreases with magnification of a degree of a strain. Three stage of plastic deformation from EPA datas is established. In table 1 the areas of a strain obtained by a method are indicated and are compared to datas obtained by a method of acoustic emission (AE).

Method	1 stage	2 stages	3 stages	4 stages
E	0 - 2.2 %	2.2 - 10.2 %	10.2 - 28 %	> 30 %
EP	0 - 3.5 %	3.5 - 10.5 %	10.5 - 19 %	

Is shown, that the method is most sensitive to the contents of defects on the first stage of plastic deformation. On this stage the vacancies and dislocations will be derivated mainly. The further growth of a strain of a sample results to increasing of concentration of defects and overwhelming number of positrons are captured on defects. Is shown, that on the second stage of plastic deformation practically all positrons annihilated from the capture on dislocations states (the parameters leave on saturation). From experimental spectra the concentration of dislocations for want of various degrees of a strain are designed. The further development of a strain results in formation of complexes of vacancies and microporous(third stage of plastic deformation). For want of it the parameters become insensitive to micropors with sizes more 50.Further magnification of voltage (more than 25 %) results in development of a crack and destruction of a material. Thus method is most informative on early stages of development of plastic deformation and allows to define for want of it concentration of dislocations.
1. C. Lopes Gill, A.P. de Lima et.al. Radiation Effects and Defects in Solids. 132, (1990) 111.
2. V.V. Korjevskij, L.P. Metlitskaia Fizika Metallov i Metallovedenie 58, (1984) 986

A6.23
ELASTIC CONSTANTS OF CUBIC ALLOY SINGLE CRYSTALS.
Craig S. Hartley, U.S. Department of Energy, Germantown, MD.

Elastic constants of single crystals are direct consequences of the nature and type of interatomic bonds in crystalline materials. Not only do they determine many properties of defects in crystals but also technologically important quantities such as the bulk modulus and Young's modulus of polycrystalline materials. These material properties thus represent one of the principal applications of multiscale modeling, where the characteristics of atoms can be related directly to the properties of bulk material through appropriate averaging procedures. Experimental data on single crystal constants is available for many elemental materials. Substantially fewer instances exist of experimental determinations of single crystal elastic constants of single phase, disordered alloys as functions of composition and temperature. Where experimental studies are not available, first principles calculations of elastic constants of elemental materials are often possible, although computationally intensive. Lattice models of crystals, consisting of atoms held together by interatomic forces extending to a limited number of neighbor shells, have proved successful in representing elastic constants as linear combinations of Interatomic force constants, defined in terms of appropriate derivatives of an interatomic pair potential. For disordered alloys, an effective interatomic pair potential can be defined as a pairwise average of the potentials characteristic of each species of atomic pair in the crystal. This effective potential can then be used in the lattice dynamics formalism to determine elastic constants of disordered alloys as functions of composition. Several examples are presented for both face-centered cubic and body-centered cubic alloys, consisting of simple metal and transition metal solutes and solvents. Estimates of elastic constants of metastable forms of elements and alloys, obtained by applying the appropriate lattice dynamics formalism to potentials determined from measurements on stable phases, are also given. Although the method is developed for modified central potentials in cubic crystals, it can be extended to angularly dependent potentials and crystals of lower symmetry by the same reasoning. The approach provides a technique for calculating elastic constants of single crystals of materials at temperatures and compositions where experimental determination is difficult or infeasible.

A6.24
ON THE INTERACTION BETWEEN POINT DEFECTS AND DISLOCATIONS. Catalin R. Picu, Rensselaer Polytechnic Institute, Department of Mechanical Engineering, Aeronautical Engineering and Mechanics, Troy, NY.

The interaction between point defects and dislocations is studied in three-dimensions in a model system, by atomistic simulations and by employing a new coupled atomistic-continuum technique. The energetic forces acting on both dislocation and point defects are computed and compared with similar results obtained by using local and non-local elasticity theory. Point defects that have been captured in the core have a different effect on the Peierels stress of the dislocation than those that stand out of it. Attention is focussed here on the influence of external defects on the mobility of the dislocation. A parallel between the description of point defect migration and that of dislocation motion is drawn. Finally, preliminary data on pipe diffusion are presented.

A6.25
DISLOCATION MOBILITY IN TWO-DIMENSIONAL LENNARD-JONES MATERIAL. Nicholas Bailey, Jeffrey Tomasi, James Sethna, Physics Dept, Cornell Univ, Ithaca, NY; Christopher Myers, Theory Center, Cornell Univ, Ithaca, NY.

In seeking to understand at a microscopic level the response of dislocations to stress we have undertaken to study as completely as possible the simplest case: a single dislocation in a two dimensional crystal. The intention is that results from this study will be used as input parameters in larger length scale simulations involving many defects. We present atomistic simulations of defect motion in a two-dimensional material consisting of atoms interacting through a modified Lennard-Jones potential. For a single dislocation at zero temperature, as a function of applied shear stress, there are transitions from no motion to a hopping motion to a steady sliding

motion. In studying the stationary → hopping transition we focus on determining whether it was hysteretic or continuous, i.e. first or second order. We also explore the behaviour as a function of all three components of the stress tensor. As well as the motion of the defect, we have studied the energy barrier to hopping when the stress is below the critical value; this barrier is relevant to the motion at finite temperature where thermally activated hopping is important. Special consideration has been given to the problem of phonons being reflected from the boundaries back towards the defect. To minimize reflections, the atoms are subject to Langevin-type damping forces. Conditions are derived to ensure that at least the dominant phonon modes are damped as completely as possible.

A6.26
JOINING OF ATOMISTIC TREATMENT AND ELASTIC CONTINUUM TREATMENT IN EDGE DISLOCATIONS.
Masao Doyama, Y. Kogure, Teikyo University of Science and Technology, Uenohara, Yamanashi, JAPAN.

The elastic continuum treatment of dislocations has always suffered from difficulties associated with the dislocation core. Expressions for the stress around a dislocation, derived by the continuum method, invariably have a singularity at the center of the dislocation. This difficulty is usually overcome by treating separately that part of the crystal which lies inside a small cylindrical core whose axis is the dislocation and radius of which is r_e. This part is refered to as the dislocation core, and the linear elastic theory is said to break down in this region. The integrations which are involved in calculations of dislocation energy use r_e as a lower limit of the radius. This procedure is unsatisfactory in that without knowing the exact arrangements of atoms in the core one has difficulty in choosing a value of r_e. there is no satisfactory way of dealing with that part of the crystal which lies inside this radius. In this paper, all atoms in the core are treated by molecular dynamic method using embedded atom potential. The results are compared with those using pair potentials, Morse potential. The cylindrical crystal near the core is embedded in a thick wall continuum cylinder and the stress and the energy was minimized, expanding the cylinder. By this way, the volume expansion could be calculated. According continuum thoery, the volume expansion cannot be treated.The treatment was also expanded to the split dislocation.

A6.27
FROM ELECTRONIC STRUCTURE TO PROPERTIES OF DISLOCATIONS: COMBINED FIRST PRINCIPLES BAND STRUCTURE AND MODIFIED PEIERLS-NABARRO MODEL ANALYSIS.
O.N. Mryasov Yu. N. Gornostyrev and A.J. Freeman, Northwestern Univ., Dept. of Phys. and Astron., Evanston, IL.

Reliable dislocation properties theory for metals, and especially for intermetallics, remains a challenge since an accurate microscopic description of inter-atomic interactions has to be combined with modeling at mesoscopic-length scales. Thus, we proposed physically transparent scheme for analyzing dislocation structure and mobility based on solution of the modified Peierls-Nabarro model with discrete representation of the misfit energy calculated by ab-initiotechniques. This scheme reveals new capabilities of the PN model concept for understanding fundamental features of dislocation behaviour and their characteristics such as (i) multiple core states and (ii) Peierls stress. We demonstrate that it is possible within this approach (i) to improve significantly agreement between theoretical estimates of the Peierls stress and experimental results; (ii) to identify reasons for disagreement between results obtained with different experimental methods; (iii) to investigate the contributions of such key factors as lattice structure, elastic anisotropy, and the peculiarities of inter-atomic interactions (γ-surface geometry and chemical bonding). All this is illustrated with realistic examples for dislocations in fcc metals (Au, Ir, Al) and intermetallic compounds $L1_0$ TiAl and CuAu and B2-NiAl with γ-surfaces calculated using ab-initio methods. We find that in agreement with experiment the unit dislocation in TiAl is compact, spread in CuAu and split in Ir and Au. The calculated dislocation structures are in good agreement with available electron microscopy measurements. The experimentally observed hierarchy of slip modes, low temperature deformation behaviour and TEM measurement in NiAl are explained. Our results shows that in this alloy elastic anisotropy and alloying effects determine observed relation between Peierls stress for edge and screw orientations. Thus, method allows to modify traditional views on dislocation core structure evolution in the process of dislocation motion and/or with external stress.

A6.28
QUANTUM TUNNELING OF DISLOCATION KINKS IN COPPER.
Siew-Ann Cheong and James P. Sethna, Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY; Tejs Vegge, Center for Atomic-scale Materials Physics, Department of Physics, Technical University of Denmark, Lyngby, DENMARK.

A number of recent experiments suggest that atomic quantum tunneling centers may occur in metals containing high densities of dislocations. Two-channel Kondo effects attributed to symmetric tunneling states have been observed in Cu, Ti, and $Fe_{80}B_{20}$, and are sensitive to the deformation history. Glassy behavior in the response of heavily dislocated aluminum has been attributed to quantum tunneling centers. Quantum dephasing of conduction electrons in metals at low temperatures has been recently attributed to scattering from tunneling systems. Kinks on dislocation lines are excellent candidates for these tunneling centers: they are naturally symmetric, and have small effective masses because the extended core structure of the defect spreads the motion among many atoms. We calculate the quantum tunneling for kinks on dislocation lines within the instanton approximation and using effective medium potentials.

A6.29
A SYSTEMATIC INVESTIGATION OF STRAIN RELAXATION, SURFACE MORPHOLOGY AND DEFECTS IN TENSILE AND COMPRESSIVE InGaAs/InP LAYERS.
Claudio Ferrari, Laura Lazzarini, Giancarlo Salviati, CNR-MASPEC Inst, Parma, ITALY; Marco Natali, Marina Berti, Davide De Salvador, Antonio V. Drigo, INFM, Physics Dept, Padova Univ, Padova, ITALY; Giacomo Torzo, Gilberto Rossetto, CNR-ICTIMA Inst, Padova, ITALY.

The strain relaxation mechanism in lattice mismatched heteroepitaxial semiconductor layers is still a matter of considerable debate. This is true in particular for layers under tensile stress which generally present a defect structure and a surface morphology much richer and complex than that of layers under compressive stress. In this work we present a systematic investigation of the strain relaxation curves and of the surface morphology as well as a characterisation of the defects in tensile and compressive MOCVD grown $InxGa_{1-x}As/InP$ layers. A large number of samples has been grown and characterised by HRXRD, RBS, SFM, TEM X-ray topography and CL covering the misfit interval from -2.3 to +1.5 percent and a range of thickness from 8 to 2400nm. In compressive InGaAs/InP layers strain relaxation is found to follow the same curve previously reported for MBE-grown InGaAs/GaAs layers despite the large difference in dislocation glide velocity. This clearly shows that relaxation is not limited by dislocation glide kinetics. Strain relaxation in tensile layers is found to be strongly asymmetric with the preferential relaxation occurring along the [110] direction. The asymmetry increases with increasing tensile misfit. The critical thickness for the onset of strain relaxation is found to be larger by a factor between 2 and 10 with respect to compressively strained layers, depending on the lattice misfit and on the [110] in-plane direction. Strain relaxation at low misfit is governed by the formation of 60 a/2< 110 > MDs while at high misfit stacking-faults and twins play a major role. Cracks are found to form after growth and are preferentially aligned along the [110] in-plane-direction as a consequence of the asymmetry of the residual strain. Grooves form in correspondence of a network of stacking-faults/twins approximately at the onset of measurable strain relaxation.

A6.30
DEFECT CALCULATIONS FOR YTTRIUM-ALUMINUM PEROVSKITE AND GARNET CRYSTALS.
Maija M. Kuklja, Electrical Engineering Department, Michigan Technological University, Houghton, MI; Institute of Chemical Physics, University of Latvia, Riga, LATVIA.

Yttrium Aluminum compounds are important materials, which technological applications range from lasers to propulsion systems. For example, the Nd^{3+} doped YAG is a well-known laser material whereas $YAG:Al_2O_3$ composite is found to be an ideal material for high-temperature ceramic applications. In the present study, theoretical simulations of basic point defects in Yttrium-Aluminum Perovskite ($YAlO_3$) and Garnet ($Y_3Al_5O_{12}$) crystals were performed in terms of interatomic potentials coupled with the classical shell model description of the lattice ions. A new set of potential parameters first obtained for the perfect lattice allows us to model atomic structures of different types of the intrinsic (vacancies, interstitials, antisites) and impurity (Ca^{2+}, Mg^{2+}, Ba^{2+}, Sr^{2+}, Cr^{3+}, Fe^{3+}, Nd^{3+}, Si^{4+}) point defects. Using calculated defect formation energies we obtain activation energies for defect reactions, from which we determine the most probable defect processes in Yttrium-Aluminum perovskite and garnet. We found that in both compounds the antisite disorder is more favorable than the Frenkel and Shottky-like disorder. It is shown that antisite substitution Y^x_{Al} causes a distortion in the crystalline lattice shortening the Y-O bond length whose calculated value is in excellent agreement with the EXAFS measurements. Deviations from stoichiometry were modeled by an excess of yttrium and aluminum oxides. Some other properties such as electrical conductivity induced by impurity defects, changes in elastic properties, and complex defect cluster formations as well as migration mechanisms were also considered. A comparison with the relevant experimental data is presented.

A6.31
PLASTICITY OF THE AlPdMn-ξ' QUASICRYSTAL APPROXIMANT. M. Feuerbacher, K. Urban, IFF, Forschungszentrum Juelich, Juelich, GERMANY; H. KLein, ESRF, Grenoble, FRANCE.

$\xi\prime$-AlPdMn is a complex intermetallic phase with 316 atoms/cell. It is an approximant of the quasicrystalline icosahedral phase in this alloy system. The structure contains Mackay-type clusters of local icosahedral symmetry as basic elements. These define a length scale, which plays an important role in the plastic deformation mechanism. We present a study on the plastic behavior of $\xi\prime$-AlPdMn. It includes deformation tests on single crystalline samples as well as microstructural characterizations of deformed material in a transmission electron microscope. Our results show that two deformation mechanisms are acting. A martensitic-type mechanism mediated by local atomic jumps and a dislocation mechanism. The interaction of these mechanisms leads to the formation of a new type of defect, the metadislocation. We will discuss the defects and the plastic behavior of this material and give a comparison with the properties of the corresponding icosahedral phase.

A6.32
MICROSTRUCTURAL MECHANICAL PROPERTIES ON A NANOMETER SCALE - NANOINDENTATION EXPERIMENTS AND FINITE ELEMENT SIMULATIONS. Mathias Göken,William D. Nix, Stanford University, Dept of Materials Science and Engineering, Stanford, CA.

The behavior of materials on a macroscopic scale is most often determined by the elastic and plastic properties of microscopically small constituents. The size of precipitated phases or grains is often smaller than a micron. In lamellar TiAl alloys, for example, extremely small lamellae with dimensions around 100 nm are desired, to optimize the macroscopic strength and fracture resistance. Simulations of the macroscopic material behavior require a knowledge of the material parameters on the length scale of these small microstructures. Nanoindentation techniques now allow a direct evaluation of the properties in the nanometer range. On this scale, anisotropic crystal plasticity plays an important role for many materials, especially intermetallic compounds, since single crystalline properties are always tested. Results of microstructural evaluations of TiAl alloys and small precipitated phases (intermetallic compounds) are presented. AFM images of impressions left by nanoindentations often show anisotropic material pile-ups around the indents, which are determined by the geometry of the crystal slip systems. A careful analysis of anisotropic effects is necessary. For many metallic materials, a significant indentation size effect is associated with ultra low load indentations. Load ranges and tip shape influences, therefore, have to be considered, too. Coupling of nanoindentation techniques with finite element modeling is very helpful for the interpretation of experiments. Yield stresses can be extracted from load-displacement curves, by comparing them with simulations. Finite element simulations of the indentation process were performed, where a small precipitate is embedded in a matrix of different material. With these simulations, the influence of the microstructure on experimental measurements could be determined, and accuracy limits of the nanoindentation method were obtained.

A6.33
ATOMISTIC SIMULATION AND EXPERIMENTAL INVESTIGATION OF ULTRA PRECISION CUTTING PROCESSES. Ruediger G. Rentsch, Laboratory for Precision Machining (LfM), Bremen University, Bremen, GERMANY.

In ultra precision machining the actual cutting process can take place at atomic level. Hence, the acquisition of many typical cutting process data is difficult or impossible. Extreme quality requirements regarding surface roughness, shape accuracy and machining process-related damage of the sub-surface layer require an effective process of control. The knowledge of the local stress state is of particular interest for functional surfaces, since high stresses can cause significant warping of the parts. Therefore, a detailed characterization and understanding of the cutting process are vital for its effective control as well as for further tool and process development. Microstructural modeling employing the molecular dynamics (MD) provides a unique opportunity to study processes and local material deformation behavior at the atomic level. Its potential for studying phenomena related to ultra precision cutting processes will be demonstrated by an approach that focuses on linking the results of atomistic simulation with results and observations from cutting experiments. A strategy of validation and evaluation of the MD model by experiments provides a basis for an extention of the modeling of cutting processes into the atomic range. Beyond common deformation and structure analysis, extended analyses allow for examination of the continuous temperature and stress distributions. This demonstrates the potential of MD to capture further microstructural information in metal processing. MD models for forging, die pressing and cutting allow, at least in principle, to extract directly information about strain, strain rates and friction conditions. Such information is useful for description of local material properties in mesoscopic and macroscopic models as well as for direct comparison with analytical and continuum mechanics models for validation and support. Some of the short-comings of the present MD modeling and possible solutions will also be discussed.

SESSION A7: FRACTURE AND CRACK PROPAGATION
Chairs: L. B. Freund and Mark F. Horstemeyer
Thursday Morning, December 2, 1999
Room 208 (H)

8:30 AM *A7.1
DISCRETE DISLOCATION ANALYSIS OF FATIGUE CRACK GROWTH. Harko Cleveringa, Alan Needleman, Brown University, Division of Engineering, Providence, RI; Erik van der Giessen, Delft University of Technology, Koiter Institute Delft, THE NETHERLANDS.

Discrete dislocation effects play an important role in crack initiation and propagation under cyclic loading, especially near the threshold regime, where a small plastic zone will form around the crack tip in which the local stress concentrations of the individual dislocations have a strong influence on whether or not decohesion will take place. This paper studies the evolution of the dislocation structure around a propagating crack tip under cyclic loading using discrete dislocations. We consider small scale yielding around a plane strain mode I crack. Hence, dislocations are confined to a region close to the crack tip while at a large distance away from the tip, tractions and/or displacements can be prescribed corresponding to the linear elastic mode I field with a stress intensity factor K. In the simulations, the value of K is varied cyclically in time with a prescribed frequency and mean value. The dislocations are all of edge character, and are modeled as line singularities in an elastic solid. The dislocations are represented using closed-form analytical solutions for the dislocation stress and strain fields in a half-plane. The boundary conditions are enforced by a complementary solution which is obtained by a finite element method. Short range dislocation interactions are incorporated into the model through a set of constitutive rules. Dislocation motion is governed by a linear drag relation so that the dislocation velocity is proportional to the Peach-Koehler force; dislocation dipoles are generated by simulating Frank-Read sources; annihilation of dislocations occurs when two opposite signed dislocations come within a critical distance, and dislocations can get locked at obstacles in the material. To model crack growth, a cohesive surface is included ahead of the crack. The traction-separation law used over this surface is motivated by atomic de-bonding.

9:00 AM A7.2
X-RAY MICROBEAM DIFFRACTION MAPPING OF DIFFERENT TEXTURE SCALES IMPORTANT IN FATIGUE CRACKING OR IN LARGE DEFORMATIONS. S.R. Stock, School of Materials Science and Eng., Georgia Institute of Technology, Atlanta, GA; and Z.U. Rek, Stanford Synchrotron Radiation Laboratory, Stanford, CA.

Polychromatic synchrotron x-ray microbeam diffraction allows one to record Laue patterns simultaneously from all of the grains within the column of material irradiated. This paper describes 3-D texture mapping in polycrystalline Al, Cu and Ti samples. Transmission methods for determining the depths of diffracting volumes are outlined. The focus is on how the texture scale between micro- (i.e., individual grain orientations) and macro-texture defines fatigue crack paths in Al-Li 2090 T8E41: very large volumes of near single crystal material lead to large asperity formation, and at least forty volume percent of the material consists of these volumes. Some results on grain subdivision in Cu after large deformations will also be covered as well as preliminary results on fatigue cracked Ti-6V-4Al.

9:15 AM A7.3
MULTIPLE SLIP-PLANE MODEL FOR CRACK-TIP PLASTICITY. S.J. Noronha, S.G. Roberts, A.J. Wilkinson, University of Oxford, Department of Materials, Oxford, UNITED KINGDOM.

Roberts and Hirsch have developed simple dislocation dynamics based models for the brittle-ductile transition based on modelling the plastic zone at a crack tip as a dislocation array emitted by a source onto a single slip plane. The models have been successful in predicting the fracture behaviour of many single crystal materials, (metals, ceramics and semi-conductors). These models requires the use of a dislocation velocity law, dislocation source activation characteristics and spacing, etc. derived from experiments for a given material. Here, we present results on iron and iron alloys. The crack-tip plastic behaviour is studied assuming different dislocation source configurations. The

effect of modelling the plastic zone as a single slip plane and as an array of parallel slip planes will be described. The effects of blocks to dislocation motion (grain boundaries, brittle precipatates) on the dislocation arrays and on crack tip behaviour will also be described. The results of the simulations will be compared with experiments.

9:30 AM A7.4
THE QUASICONTINUUM METHOD: APPLICATIONS TO MATERIALS WITH COMPLEX CRYSTAL STRUCTURES.
Nitin Bhate and Rob Phillips, Division of Engineering, Brown University, Providence, RI; Ronald Miller, Department of Mechanical Engineering, University of Saskatchewan, CANADA.

The quasicontinuum method is a finite element based mixed atomistic-continuum technique where the constitutive response of the material is derived from atomistic calculations. The quasicontinuum method has recently been extended to simulate the response of complex crystal structures described by a Bravais lattice with a basis. In these materials, a macroscopically uniform strain will not necessarily lead to uniform atomic displacements, as different basis atoms can rearrange with respect to each other to further reduce the total energy. The quasicontinuum method can now be used effectively to study the material response of complex lattices as well as ordered compounds. In this paper, we describe the application of this technique to investigate stress-induced phase transformations and fracture in Zr and Ni-based ordered alloys. Zr has been known to undergo bcc (simple Bravais lattice) to hcp (complex Bravais lattice) phase transformation. Ni-based ordered alloys readily undergo stress induced transformations, making them a common material for shape memory applications. The method allows us to investigate the kinematics of phase transformations under non-uniform, multiaxial loading conditions, and in regions of high stress such as around a crack tip.

10:15 AM A7.5
PERCOLATION THEORY OF DISLOCATION TRANSPORT IN DEFORMED METALS.
Robb Thomson (Emeritus) and Lyle Levine, Materials Science & Engineering Laboratory, National Institute of Standards and Technology, Gaithersburg, MD.

We have previously reported an application of percolation theory to the problem of dislocation transport in deformed metals where a well developed dislocation cellular structure is present. This paper discusses further developments. A sum rule and mean field approximation have been derived in 2D which predict that the deforming metal is a self organizing system. The strain percolation problem is a type of correlated percolation, whose percolation threshold is sensitive to which of several possible paradigms are chosen. But for all paradigm choices, the universality class is the same as that of standard percolation theory. The mean field approximation predicts a critical line for the system in the parameter space governing the stochastic strain transmission law, which depends on only two independent parameters. However, the numerical simulations show that the critical line spreads into a surface in 3D parameter space. The details of this critical surface will be presented. Finally, we discuss the implications of the mathematical model for actual deforming metal systems.

10:30 AM A7.6
DAMAGE AND FRACTURE AT A MICROSTRUCTURAL SCALE.
Elisabeth Bouchaud, SRSIM, Gif-sur-Yvette Cedex, FRANCE; Florin Paun, DMMP, ONERA, Chatillon Cedex, FRANCE; Elodie Ducourthial, DMSE, ONERA, Chatillon Cedex, FRANCE.

The self-affine morphology of fracture surfaces retaining both universal and microstructure-dependent aspects has attracted a great interest these last few years. An attempt to interprete fracture of heterogeneous materials as a dynamic phase transition has been made. If models of fronts moving through randomly distributed microstructural obstacle forces have given satisfactory qualitative results, they failed to predict the actual experimental observations quantitatively. One of the main weaknesses of this category of models is that they do not take damage into account. The central point of the work presented here is to show the relevance of damage in this context. The morphology of damage cavities has been analysed with an Atomic Force Microscope on various aluminium alloys. It is shown that the roughness of small cavities which have not joined with the main crack corresponds to the small length scales self-affine regime observed on fracture surfaces. This roughness is different from the roughness of bigger cavities constituted by the coalescence of smaller ones. On the other hand, it is argued on the basis of both experimental and numerical results that the self-affine correlation length of fracture surfaces is a damage correlation length, depending on microstructure, external load and crack velocity. These various conclusions suggest a new scenario for crack propagation, based on the nucleation and coalescence of damage cavities.

10:45 AM A7.7
TEMPERATURE EFFECTS AND CRACK PROPAGATION AT HIGH STRAIN RATE DEFORMATIONS.
E.D. Metselaar, A. Roos, J.Th.M. De Hosson, Department of Applied Physics, Materials Science Centre and Netherlands Institute for Metals Research, University of Groningen, Groningen, THE NETHERLANDS; H.H.M. Cleveringa, E. Van der Giessen, Delft University of Technology, Delft, THE NETHERLANDS.

During the deformation process mechanical energy is converted into heat. The temperature rise may trigger thermal softening and shear instability, which will occur at smaller strain with increasing strain rate. Depending on the thermo-physical properties like the thermal diffusion length the flow stress may decrease rapidly with respect to neighboring regions. This will tend to localize the deformation even more. This work extends a computer simulation methodology based on the framework of discrete dislocation plasticity. The paper concentrates on modeling of the temperature rise due to a fast moving crack in a material with a high thermal conductivity, e.g. Al and a material with a low thermal conductivity, e.g. Ti. Based on linear fracture mechanics it can be shown that the temperature rise of a running crack in Ti at half the Rayleigh velocity can attain 2000 0 K. In the discrete dislocation plasticity approach the crack was described by a distribution of a double pile-up of dislocations as was put forward by Eshelby, Nabarro, Bilby and Leibfried in the past. A one micron crack in Al was represented by using approx. 500 dislocations and by 114 in Ti. It was concluded that the local heating as experimentally is observed in Ti-alloys has to do with fast moving cracks rather than with fast moving dislocations. The former leads to a considerable localised heating whereas in the case of moving dislocations the temperature rise was too small.

11:00 AM A7.8
SCALING EFFECTS IN THE DUCTILE TEARING RESISTANCE OF METALS.
Otmar Kolednik, Karl H. Ziehenberger, Christian Stachelberger, Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, AUSTRIA; F.D. Fischer, Institute of Mechanics, University of Leoben, AUSTRIA.

This investigation is devoted to the variation of the crack growth resistance in fracture mechanics specimens when the specimen type, size and geometry are altered. With analytical considerations, stereophotogrammetric measurements and finite element modeling the main influence factors on the scaling effects are deduced: These are the effects of the in-plane and the out-of-plane constraint on both the fracture behavior and the global deformation behavior of the material. The fracture behavior is governed by the conditions prevailing within the process zone (Q-stresses, stress triaxiality) which determine void initiation, void growth and coalescence directly in front of the crack tip. Stereophotogrammetric studies have been conducted, applying a recently developed digital image processing system for the automatic analysis of stereo image pairs taken in the scanning electron microscope. This system provides a three-dimensional model of the depicted fracture surface region consisting of about 10000 to 20000 points. The variations of the critical crack tip opening displacement (COD_i) and the critical crack tip opening angle (CTOA) have been determined as a function of the distance from the specimen side surfaces. This was done for specimens with a high in-plane constraint, i.e., a Compact Tension (CT) specimen, as well as for a specimen with a low in-plane constraint such as a Center Cracked Tension (CCT) specimen. Finite element computations have been made to study the effects of the in-plane and out-of-plane constraint on the deformation behavior. It is demonstrated that even for CT specimens under plane strain conditions the global deformation behavior and, consequently, the crack growth resistance, of specimens may change with varying crack length over width (a/W) ratio, although the Q-stresses or the stress triaxiality within the process zone are constant. For bend-type specimens under large-scale yielding conditions the ratio specimen thickness over ligament length has been found to determine the deformation behavior.

11:15 AM A7.9
VOID SHAPE AND VOID DISTRIBUTION EFFECTS ON COALESCENCE IN ELASTIC-PLASTIC SOLIDS.
Thomas Pardoen and John W. Hutchinson, Harvard University, Division of Engineering and Applied Sciences, Cambridge, MA.

Successful application of void growth based plastic constitutive models for ductile failure analysis relies on the way the relevant microstructural input is accounted for. State of the art approaches used in metal forming modelling and for integrity assessment of cracked or non-cracked structural components typically require (1) the initial porosity, (2) one internal length related to the void spacing, (3) a critical porosity for cracking initiation, (4) a critical porosity for final failure, and (5) nucleation parameters (when this stage is taken into account). The present study shows that, in order to be valid in both low and high stress triaxiality regime, i e from uniaxial to crack

tip fracture process zone stress states, void shape effects have to be incorporated in the void growth-coalescence models. Void shape is also an important issue when looking at materials with nucleation sites whose initial shape significantly departs from spherical. A model for the coalescence of voids is proposed and assessed using void cell simulations. In an extension of Thomason's ideas, this model directly addresses the mechanism of coalescence by tensile localisation of plastic deformation in the intervoid ligament. The onset of coalescence depends on the current void shape, void spacing, porosity, and average yield stress of the base material. Evolution laws for all these parameters and for the stress after the onset of coalescence are derived from simple geometrical and mechanical arguments. Prediction of cracking initiation as well as of the final drop of the load carrying capacity of the material are thus obtained without introducing a phenomenological critical porosity. The assessment of the model was performed for various initial porosity for prolate and oblate voids, for different void spacing ratios, and for various strain hardening exponents.

11:30 AM A7.10
NUMERICAL MODELING OF VOID GROWTH AND COALESCENCE IN NICKEL. P. David Pattillo II, Univ of Illinois, Dept of Theoretical & Applied Mechanics, Urbana, IL; Brian P. Somerday and Mark F. Horstemeyer, Sandia National Laboratories, Materials & Engineering Sciences Center, Livermore, CA.

Face-centered cubic alloys typically fracture by the nucleation, growth, and coalescence of voids. Experimental efforts have identified the mechanisms for microvoid nucleation, growth, and coalescence and have characterized the mechanical and microstructural variables that affect the fracture mode. Complementary studies to model microvoid fracture are not as extensive. The objective of this work is to improve the predictive capability of numerical void-damage models by including the effects of applied strain, strain rate, hydrostatic stress, temperature, void distribution, dissolved hydrogen, and microstructure. Atomistic simulations of void growth and coalescence are emphasized and comparisons with micromechanical finite-element results are included. Energy minimization and molecular dynamics simulations are conducted using the Embedded-Atom Method on lattices of nickel containing cylindrical voids. The growth and coalescence of voids are assessed as a function of strain, strain rate, hydrostatic stress, and void distribution. Interstitial hydrogen is introduced into the lattice to determine whether this element accelerates void growth and coalescence.
(*This work is supported by the U.S. Dept of Energy under contract # DE-AC04-94L85000.)

SESSION A8: DISLOCATION-INTERFACE INTERACTIONS
Chairs: Ian M. Robertson and Anthony D. Rollett
Thursday Afternoon, December 2, 1999
Room 208 (H)

1:30 PM *A8.1
THE STRUCTURE AND MOBILITY OF DEFECTS FORMED BY ABSORPTION OF CRYSTAL DISLOCATIONS IN INTERFACES IN THE HCP METALS. D.J. Bacon, R.C. Pond and A. Serra*, Materials Science and Engineering, Department of Engineering, The University of Liverpool, Liverpool, UNITED KINGDOM; *Department de Matematica Aplicada III, Universitat Politecnica de Catalunya, Barcelona, SPAIN.

Atomic-scale computer simulation techniques have been used to investigate the interaction of crystal dislocations with the {10-12} twin boundary and a <1-210>/90° tilt boundary in the HCP metal α-titanium. The latter interface is incommensurate in the direction perpendicular to the tilt axis. Crystal dislocations are always found to be absorbed in the tilt boundary with concomitant reconstruction of their cores. In the twin boundary, a broader range of interactions is observed, including defect transmission from matrix to twin and decomposition in the interface into discrete defects. The simulations demonstrate that the core structures of localised interfacial defects exhibit preferred riser structure. For the twin, it is the 'basal-on-prism' configuration, whereas risers in the tilt boundary resemble {10-12} twin forms. By comparing interaction processes in two interfaces, the role of crystallographic considerations and interfacial structure has been elucidated. In response to applied shear stress, interfacial defects with Burgers vector, b, parallel to their host interface can move conservatively in principle, but are mobile only if their step height, h, is small and their core is wide. Conversely, defects which exhibit large h generally have narrow cores and require complex shuffles for motion: applied stress tends to cause core reconstruction of these defects. Defects with b inclined to the interface can move conservatively in some circumstances in response to stress through a climb-compensated mechanism. This can lead to limited mobility of defects in both types of interface, and involves the generation of additional glissile interfacial defects due to the stress concentrating effect of the riser of the initial defects. Activation of this mechanism is only feasible when the elementary mechanism of motion involves a small number of atoms shuffling from one crystal to the other, but is not simply related to h and can occur even when h is relatively large.

2:00 PM A8.2
DISLOCATION INTERACTIONS WITH GRAIN BOUNDARIES IN LAMELLAR TITANIUM ALUMINUM INTERMETALLICS. Jorg M.K. Wiezorek, University of Pittsburgh, Department of Materials Science and Engineering, Pittsburgh, PA; Xiao-Dong Zhang, Reynolds Metals Company, Chester VA; Hamish L. Fraser, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH.

Two-phase TiAl based intermetallics with microstructures comprising large volume fractions of lamellar grains are promising candidate materials for applications in advanced jet-engines. The anisotropic mechanical properties associated with the lamellar microstructure are very well documented in the literature and so-called soft and hard deformation modes can be distinguished. The boundaries between neighboring gamma-TiAl lamellae and alpha-Ti_3Al and gamma-TiAl have been proposed as very efficient obstacles for dislocation motion during hard mode deformation and supposedly, play an important role in strengthening of lamellar TiAl. The present experimental study investigates defect interactions with these lamellar interfaces which have become the basis for models describing the strength of lamellar TiAl alloys. The details of shear transfer across lamellar boundaries between gamma-variants and across phase boundaries have been identified and the processes for activation of slip in the less ductile alpha-Ti_3Al lamellae have been elucidated. Thus the role of defect interactions with lamellar interfaces on the strength and ductility of two-phase TiAl has been assessed. Part support for this work by a grant from the National Science Foundation with Dr. Bruce MacDonald as program manager is gratefully acknowledged.

2:15 PM A8.3
OBSERVATION AND MODELING OF GRAIN BOUNDARY DISLOCATION STRUCTURE AND BEHAVIOR. D.L. Medlin and S.M. Foiles, Materials and Engineering Sciences Center, Sandia National Laboratories, Livermore, CA.

An important step to incorporating grain boundaries into multiscale materials models is including the effects of interfacial dislocations. In this presentation, we discuss atomistic and continuum models for grain boundary dislocations and relate these models to experimental observations made by high resolution and in situ transmission electron microscopy. We focus primarily on dislocations present at boundaries in the FCC Σ=3 system. Though crystallographically a simple geometry, the interfacial dislocations present in this system, which have Burgers vector of either 1/3< 111 > or 1/6< 112 >, exhibit a rich variety of structural relaxations and dynamic behavior that depend sensitively on the boundary orientation. From an experimental and computational analysis of the local atomic scale relaxations in the vicinity at such defects, we provide insight into the larger length-scale coupling of interfacial dislocation motion, by both glide and climb processes, with grain boundary motion. This work is supported by the U.S. Department of Energy under contract DE-AC04-94AL85000, in part by the Office of Basic Energy Sciences, Division of Materials Science.

2:30 PM A8.4
ATOMISTIC SIMULATIONS OF DISLOCATION-INTERFACE INTERACTIONS IN THE Cu-Ni MULTILAYER SYSTEM. S.I.Rao* and P.M.Hazzledine*, Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/MLLM, Wright-Patterson AFB, OH; *UES Inc., Dayton, OH.

Experimental results show that a nanolayered composite structure made of two kinds of metallic materials strengthens dramatically as the layer thickness is reduced.This strengthening can be attributed, in epitaxial systems, to four kinds of dislocation-interface interactions: modulus, lattice parameter, gamma surface and slip plane mismatches between adjacent layers. The modulus mismatch introduces a force between a dislocation and its image in the interface. The lattice parameter mismatch generates coherency stresses and mismatch dislocations which interact with a mobile dislocation. The gamma surface mismatch results in core energy changes as the glide dislocations approach the interface. Slip plane mismatch across the interface requires mobile dislocations in the screw orientation to cross-slip. In this manuscript the embedded atom method (EAM) is used to study atomistically, all four types of dislocation-interface interactions in the Cu-Ni multilayer system. It is shown that the blocking strength of the Cu-Ni interface due to all four types of interactions is significant and range in value from 0.004 to 0.05G.

3:15 PM A8.5
ATOMISTIC MODELING OF INTERFACIAL DIFFUSION IN THE LAMELLAR L10 TiAl. M. Nomura[1], D.E. Luzzi[1], V. Vitek[1], A. Landa[2] and M. Sob[3]. [1]Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA; [2]Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA; [3]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, CZECH REPUBLIC.

In recent years the lamellar TiAl with L10 structure has been identified as a very promising high-temperature structural material owing to its relatively high ductility and toughness at ambient temperatures. At high temperatures the physical and mechanical properties of materials are commonly linked with diffusion and thus knowledge of the diffusion mechanisms in TiAl is essential for a fundamental understanding of the properties of this compound. In general, diffusion is usually appreciably faster at interfaces than in the bulk and since the density of interfaces in the lamellar g-TiAl is high, the interfacial diffusion is likely to dominate. Atomistic simulation using many-body central-force potentials was utilized to elucidate the diffusion mechanisms both in the bulk and at lamellar interfaces assuming a vacancy mechanism. First the self diffusion of Ti and Al has been studied. The simulations were then extended to investigate the diffusion of molybdenum in g-TiAl. The corresponding interactions between Mo and Ti and Mo and Al were described by many-body central force potentials constructed by fitting ab initio calculated data for simple structures. The findings of this study will be discussed in relation to the experimental results of the TEM studies of the same system. This research was supported in part by the National Science Foundation grant no. DMR96-15228

3:30 PM A8.6
MECHANISMS FOR SELF-DIFFUSION IN HIGH-ANGLE TILT BOUNDARIES IN FCC METALS. Mads R. Sørensen and Arthur F. Voter, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM; Yuri Mishin, Department of Materials Science and Engineering, Virginia Tech, Blacksburg, VA.

Grain boundary self-diffusion in high-angle tilt grain boundaries in fcc metals has been studied using atomistic computer simulations with semi-empirical potentials. The key problem is to identify the dominant atomic mechanisms of diffusion. To this end, high-temperature, "basin-constrained" molecular dynamics simulations with automatic detection of transitions have been used to scan for diffusion processes. For the $\Sigma = 5$ (210) and (310) [001] symmetrical tilt boundaries in copper, we find vacancy mechanisms, interstitialcy mechanisms, and "ring-like" mechanisms, some of which have not been known previously. The rates of elementary atomic processes involved in these mechanisms have been calculated as functions of temperature within harmonic transition state theory, and used as input to a kinetic Monte Carlo model. From kinetic Monte Carlo simulations, diffusion coefficients have been determined for different directions in the boundary plane. The results are compared with experimental data obtained by the radiotracer technique.

3:45 PM A8.7
STRUCTURE AND STABILITY OF GRAIN BOUNDARIES IN MOLYBDENUM WITH SEGREGATED CARBON IMPURITIES. R. Janisch, T. Ochs, C. Elsaesser, Max-Planck-Institut fuer Metallforschung, Stuttgart, GERMANY.

The mechanical behaviour of metals, e. g. the intergranular brittleness of polycrystals, can be influenced strongly by impurities segregated to grain boundaries. In the present work, the segregation of interstitial impurities to symmetrical tilt grain boundaries (STGB) in body-centered cubic transition metals is investigated. By means of ab-initio total-energy, atomic-force and electronic-structure calculations based on the local density-functional theory, segregation energies as well as changes in atomic and electronic structures at a $\Sigma 5$ (310) [001] STGB in Molybdenum caused by segregated interstitial Carbon impurities are investigated and compared to ab-initio results for a clean $\Sigma 5$ (310) [001] STGB [1]. Energetic stabilities and structural parameters for crystalline Molybdenum Carbides with tetragonal or hexagonal symmetries and compositions MoC or $MoC_{1/2}$, are reported. Perspectives for large-scale atomistic simulations (e. g. molecular dynamics) of Carbon segregation to Molybdenum grain boundaries with empirical interatomic potentials derived from the ab-initio data are discussed. This theoretical study is motivated by recent high-resolution transmission electron microscopy (HRTEM) experiments [2], which showed the formation of segregated MoC_x intergranular films with hexagonal or tetragonal structures along $\Sigma 5$ (310) [001] STGB in Molybdenum. [1] T. Ochs et al., Phil. Mag. A (1999), in press. [2] J. M. Penisson et al., Phil. Mag. A 73, 859 (1996).

4:00 PM A8.8
INFLUENCE OF GRAIN BOUNDARY AND INTERFACE STRUCTURE ON LIQUID METAL PENETRATION BEHAVIOR. Liping Ren, D.F. Bahr, R.G. Hoagland, Washington State University, Department of Mechanical and Materials Engineering, Pullman, WA.

Liquid metal embrittlement (LME) is the reduction in elongation to failure that can occur when normally ductile metals or alloys are stressed while in contact with certain liquid metals. In severe cases, the LME failure can occur even under no applied stress condition and is usually time-dependent, e.g. Ga embrittles Al in stress-free condition. Several mechanisms have been proposed but still not been well established. To understand the time-dependent LME failure, it is critical to understand the liquid penetration behavior on different grain boundaries and interfaces. In the present study, Ga penetration behavior on Al grain boundaries and Al/Cu interfaces is investigated. High purity Al was used for examining grain boundary orientation effects on Ga penetration rates. Cu was deposited via sputter deposition onto single crystal Al to examine the wetting behavior of Ga on a Cu/Al interface. Penetration rates were measured by in-situ TEM and SEM observation for several differently oriented grain boundaries and interfaces. Molecular dynamics simulations have been conducted to explore the effects of various interface properties including interface energy, excess volume and grain boundary structure. These calculations involve interfaces with misorientations in the experiments by SEM electron channeling patterns or Kikuchi patterns of TEM diffraction. The experimental penetration rates on micro and macroscale are related to the atomistic simulations. The support of the US Department of Energy through grant DE-FG06-87ER45287 is gratefully acknowledged.

4:15 PM A8.9
ATOMISTIC SIMULATIONS OF GRAIN GROWTH. A.J. Haslam, S.R. Phillpot and D. Wolf, Materials Science Division, Argonne National Laboratory, Argonne IL.

We have performed molecular-dynamics simulations of grain growth in a three-dimensional columnar Pd polycrystal. First, however, to establish that a grain size of only ~10nm indeed captures the physics of a coarse-grain microstructure, we have tested the validity of the Herring relationship between the dihedral angles (at which grain boundaries meet at triple lines) and the GB energies. For that purpose, we started with a microstructure of identical grains of perfectly hexagonal columns (periodically repeated along their axes) with the 120-degree dihedral angles that would be present in an equilibrated microstructure if the GB energies were isotropic. Because the GB energies are actually anisotropic, upon equilibration we observed significant deviations from 120-degree dihedral angles, consistent with the Herring relation and with recent experiments. Our grain growth simulations used an equilibrated initial microstructure with a log-normal grain-size distribution of typically fifty grains. The time dependence of this distribution allowed us to compare with the scaling laws obtained from experiments and from mesoscale simulations. These simulations also provided atomic-level insight into the mechanisms controlling grain growth. Moreover, they allowed the determination of GB properties needed as input to physics-based mesoscale simulations of grain growth and will act as benchmarks against which to compare the results of such simulations. Work supported by U. S. Department of Energy, BES-Materials Science under Contract No. W-31-109-Eng-38.

4:30 PM A8.10
DIRECTIONAL GRAIN BOUNDARY TRIPLE JUNCTION MOBILITIES : AN ATOMISTIC SIMULATION STUDY. Moneesh Upmanyu[1], David J. Srolovitz[1,2], Lasar S. Shvindlerman[3,4] and Guenter Gottstein[4]; [1]Department of Materials Science & Eng., University of Michigan, Ann Arbor, MI; [2]Princeton Materials Institute, Princeton University, Princeton, NJ; [3]Institute of Solid State Physics, Russian Academy of Sciences, Moscow district, RUSSIA; [4]Institut fur Metallkunde und Metallphysik, RWTH, Aachen, GERMANY.

We present molecular dynamics simulations of the migration of triple junctions formed by the intersection of a straight, symmetric tilt boundary with the apex of a half-loop grain, for various triple junction grain boundary misorientations. The dynamic triple junction angle, measured as the half-loop retracts, provides a measure of the grain boundary triple junction mobility. Additional simulations are performed using a geometery where identical triple junctions move in the opposite directions (involving the destruction of the symmetrical tilt boundary, which now forms the sides of the half loop). We find that the triple junction mobility can be different depending on the direction of its motion. The triple junction migration is found to be strongly directional for triple junctions which significantly affect (drag) grain boundary migration, i.e. when the dynamic angle is significantly different from the static angle (triple junctions with low sigma grain boundaries). The variation of the triple junction mobilities with temperature is also presented. For low temperatures, the triple junction migration is found to be an activated process.

4:45 PM A8.11
TWINNING DEFORMATION IN MARTENSITE MICRO-STRUCTURE. Udomsilp Pinsook, Graeme Ackland, the University of Edinburgh, Dept of Physics and Astronomy, Edinburgh, SCOTLAND.

We employ molecular dynamic to study twinning deformation in a martensite microstructure obtained from rapid cooling β zirconium through the bcc-hcp transition. The microstructure is composed of $(10\bar{1}1)$ twin boundaries and boundary dislocations which sometimes spread across the twins forming stacking faults. A series of such equilibrium microstructures subjected to discrete, increasing $< 11\bar{2}3 > (10\bar{1}1)$ shear strain. The stress-strain curve has stick-slip behaviour with yield stress of $\approx$ 5.0Kbar and yield strain of $\approx$ 3.8%. Deformation occurs through twinning dislocations: straight perfect twin boundaries do not move.

SESSION A9: POSTER SESSION:
GRAIN BOUNDARY SIMULATIONS
Chairs: David J. Bacon and David E. Rodney
Thursday Evening, December 2, 1999
8:00 P.M.
Exhibition Hall D (H)

A9.1
TIGHT-BINDING MOLECULAR DYNAMICS MODELING OF IMPURITY ATOM-GRAIN BOUNDARY INTERACTION IN DIAMOND. Michael Sternberg, Thomas Frauenheim, Dept of Physics, University of Paderborn, Paderborn, GERMANY; Peter Zapol, Larry A. Curtiss, Dieter M. Gruen , Materials Science and Chemistry Divisions, Argonne National Laboratory, Argonne, IL.

We have studied impurity atoms in the high-angle (100) twist grain boundaries of diamond using the density-functional based tight-binding (DFTB) molecular dynamics technique with self-consistent charge extensions. The method permits us to investigate the local electronic structure and coordination of the impurity atom in the grain boundary region which is represented by a large periodic unit cell of more than 200 atoms. The study is motivated by recent progress in nanocrystalline diamond growth. Structural relaxation calculations were carried out for several grain boundaries and for different configurations of the impurity atom in the grain boundary. Various impurity atoms including hydrogen, lithium, nitrogen and silicon were studied. The low-energy atomic structures and their electronic properties are reported, and we conclude that interfacial impurities in nanocrystalline diamond increase the coordination of carbon atoms near the interface, thus playing an important role particularly in the electronic properties of diamond films. (Work supported by the U.S. Department of Energy, BES-Materials Sciences, under Contract W-31-109-ENG-38.)

A9.2
A THEORETICAL STUDY OF A VACANCY IN ALUMINUN GRAIN BOUNDARY. Gang Lu, Nicholas Kioussis, California State University Northridge, Dept. of Physics, Northridge, CA.

We present a detailed study of the interaction between a single vacancy and the Σ 5 tilt grain boundary in aluminum, based on the first-principles pseudopotential plane-wave total energy calculations. The formation energy of a single vacancy at all possible atomic sites within the grain boundary region as well as that in the bulk aluminum are calculated. We find that the vacancy formation energy at the grain boundary is not always lower than that in the bulk, in fact, it depends on the local atomic environment of the grain boundary in which the vacancy is present. It is found that the grain boundary energy could be significantly reduced by introducing a vacancy at the appropriate site of the grain boundary. We study the grain boundary sliding behavior and the corresponding electronic structure with a vacancy and without a vacancy. We find that the grain boundary sliding could be greatly facilitated if a vacancy is formed during the process of the boundary sliding.

A9.3
EFFECTIVE GRAIN BOUNDARY HAMILTONIAN FOR COMPLEX TILT BOUNDARIES. D.N. Pawaskar[1], R. Miller[2], R. Phillips[1]; [1]Division of Engineering, Brown University, Providence, RI; [2]Department of Mechanical Engineering, University of Saskatchewan, Saskatoon, CANADA.

We investigate the atomic-level structure of long-period tilt grain boundaries in aluminum using lattice statics calculations. We have built a database of structures and corresponding energies of both high and low sigma boundaries and have compared our results with those obtained using the structural unit model. Our investigation shows that for certain boundaries a revision of the structural unit paradigm may be necessary. To this end, we introduce the concept of an effective grain boundary hamiltonian which is based on energetic interactions between the individual structural units.

A9.4
MICROSTRUCTURALLY INDUCED FAILURE EVOLUTION AND GLOBAL FAILURE IN POROUS CRYSTALLINE AGGREGATES. W.M. Ashmawi, M.A. Zikry, North Carolina State University, Department of Mechanical and Aerospace Engineering, Raleigh, NC.

A multiple-slip dislocation-density based constitutive formulation and specialized computational schemes have been developed to characterize material failure on the appropriate physical scales needed for the accurate understanding and prediction of the underlying physical mechanisms that control void failure initiation, growth, and coalescence in porous crystalline aggregates. Dislocation-density transmission and blockage interfacial conditions and local stress fields have been obtained for grain-boundary distributions associated with random and low and high angle tilt and twist orientations. These evolving discontinuity and local stress fields are used as failure criteria to track the initiation and evolution of failure modes such as shear-strain localization, and intergranular and transgranular fracture in porous polycrystalline aggregates. The interrelated effects of grain boundary orientation, dislocation pile-ups, dislocation density evolution, geometrical and thermal softening, void distribution and geometry, and hydrostatic stresses on failure paths and ligament damage in cubic crystalline materials have been studied. Based on the present analysis and on comparison with experimental studies and observations, it is shown transgranular and intergranular failure can be characterized in terms of the material competition between the strengthening and the softening mechanisms of the crystalline structure. Furthermore, this investigation underscores the need to accurately account for grain-boundary effects and other interfacial conditions in crystalline aggregate formulations pertaining to failure.

A9.5
INTERACTION OF POINT DEFECTS WITH GRAIN BOUNDARIES IN INTERMETALLIC COMPOUNDS. Yuri Mishin, Dept of Materials Science and Engineering, Virginia Polytechnic Institute, Blacksburg, VA.

A statistical model of thermal and compositional disorder in grain boundaries of ordered intermetallic compounds is presented. The model is based on the approximation of non-interacting point defects and assumes thermodynamic equilibrium between the grain boundary and the bulk. Specific calculations are carried out for B2 NiAl and L10 TiAl as model systems. The free energies of defect formation are calculated using embedded-atom potentials, molecular statics, and the quasi-harmonic approximation. Form the obtained occupation probabilities of vacancies and antisite defects at different sites in the grain boundary core, the "self-segregation" characteristics are calculated as functions of temperature and bulk composition for a few boundaries. The model predictions are compared with the results of Monte Carlo simulations. Two possible mechanisms of bulk disorder are considered: the triple-defect mechanism (NiAl) and the antisite-disorder mechanism (TiAl). It is shown that the bulk mechanism of disorder does not necessarily have to dominate in grain boundaries. The effect of bulk off-stoichiometry on grain boundary properties, such as cohesive strength and diffusion, is analyzed.

A9.6
MONTE CARLO INVESTIGATIONS OF A Σ 5 TILT GRAIN BOUNDARY IN ALUMINUM. Peter Ballo, Slovak Technical University, Dept. of Physics, Bratislava, SLOVAK REPUBLIC; Nicholas Kioussis, Gang Lu, California State University Northridge, Dept. of Physics, Northridge, CA.

The microscopic mechanism for the sliding of the Σ 5 grain boundary (GB) in aluminum has been investigated at elevated temperatures. Computer simulations were performed using the finite-temperature Monte Carlo technique based on the embedding atom (EAM) potential. All calculations were performed within the canonical ensemble, using the standard Metropolis algorithm. Computed GB energy was found in a good agreement with experimental as well as ab initio data. This result shows that the appropriately fitted EAM potential can be used to predict reliable GB structures. The discontinuous changes of the GB energy at certain sliding distances are associated with the GB migrations. We find that not only one but multiple GB migrations happens during the entire GB sliding process. It is evident that in aluminium the GB migration depends sensitively on the annealing temperature. The combined motion of the GB (sliding and migration) is mediated by the thermally activated flow of the nearest neighbour atoms along the interface.

A9.7
SIMULATION ON INTERACTION OF DISLOCATIONS WITH GRAIN BOUNDARY. Yoshiyuki Kaji, Japan Atomic Energy Research

Institute, Tokai, JAPAN; Futoshi Shimizu, Hideo Kaburaki, Japan Atomic Energy Research Institute, Tokyo JAPAN; Yoshiaki Kogure, Teikyo University of Science & Technology, Yamanashi, JAPAN.

Dislocation interaction and configuration of piled up dislocations near a crystal surface or a grain boundary under external stresses are simulated by means of elastic continuum model. A purpose of the present simulation is to investigate the fundamental mechanism of Hall-Petch relation. According to the relation the dislocation pile up is considered to determine the crystal strength when the grain size is larger than a critical value. As an initial condition screw or edge dislocations of same sign are arranged in some slip planes of a crystal cell. The dislocations interact each other through the Peach-Koehler force $\mathbf{F}/L = \mathbf{b} \cdot \sigma \times \xi$, where L is the dislocation length, σ is the stress tensor produced by interacting dislocations, $\mathbf{b}$ is the Burgers vector, and ξ is a unit vector along the dislocation line. As the dislocation stress field has long range nature ($\propto 1/r$), the periodic boundary condition cannot be adopted. A dislocation also interacts with the miller dislocation at the surfaces when the fixed boundary condition is adopted. By the application of external stress the dislocation are pushed to a crystal boundary and balance with the boundary force. To obtain an equilibrium configuration the force acting on each dislocation is calculated and the atom is displaced by a distance proportional to the force component in slip plane. The process is repeated until the forces acting on every dislocation decrease under a criterion. For a tilt boundary the dislocation model is adopted, namely, the boundary is represented by an array of immobile edge dislocations and the interaction of edge dislocations is calculated. The simulation are performed for the several sizes of grains and strength of the crystal is evaluated from the maximum stress at the grain boundary.

A9.8
GRAIN BOUNDARY STRUCTURE AND TRIPLE JUNCTIONS IN COMPUTER SIMULATED NANOCRYSTALLINE FCC METALS. Diana Farkas, Virginia Tech, Dept. of Materials Science, Blacksburg, VA; Helena Van Swygenhoven, Paul Scherrer Institute, Villigen, SWITZERLAND; Alfredo Caro, Centro Atomico Bariloche, ARGENTINA.

We present a detailed crystallographic study of the structure of randomly generated grain boundaries in nano-crystalline Cu and Ni, relaxed using molecular dynamics. The results show that the grain boundaries are not amorphous-like. On the contrary, we have found many boundaries with structures that correspond to the standard models for grain boundaries in larger grain polycrystals. Low angle grain boundaries are composed of arrays of dislocations. For high angle boundaries we found similar arrays of dislocations that accommodate deviations from low sigma coincident lattice misorientations. We compared the boundary structure for samples created with the same random misorientations and grain sizes varying from 5 to 12 nm. The boundary structures are very similar for all grain sizes studied, with the smaller grain sizes containing less repetitions of the structural units composing the boundary. Our results show that the grain boundaries in nano-crystalline materials have many structural features that are expected in boundaries in larger grain materials. The implication of the observed grain boundary structure for the deformation behavior of nanocrystalline metals is discussed.

A9.9
MODELING OF THE DISLOCATION FORMATION AT PORES AND INCLUSIONS UNDER THERMO-MECHANICAL SHEAR LOADS. Ruediger Rentsch[1], Vaclav Vitek[2]; [1] Lab. f. Precision Machining (LfM), Bremen Univ., Bremen, GERMANY; [2]Dept. of Material Science and Engineering, Univ. of Pennsylvania, Philadelphia, PA.

Unlike the single crystalline structures often used in atomistic studies, real materials that form the basis for the design of engineering components contain a broad variety of defects. Such defects are grain boundaries, different phases, dislocations, pores, inclusions, and also alloying elements and impurities. Materials used in many technical applications possess a certain degree of porosity, in particular sintered materials, or heterogeneous structures, for example, due to the presence of carbides as hard inclusions. In both metals and ceramics, pores and inclusions influence significantly the elastic and plastic response. They can limit or broaden the range of applicability of the materials for high performance components and play, therefore, a very significant role in engineering applications. In manufacturing enginnering, which is concerned with the machining of materials to produce the required quality and shape of technical components, the machinability of materials, that is controlled by the ability to plastically deform, is the most important criterion. The fundamental requirement for high ductility is the ability to generate dislocations on a massive scale. Hence this study focuses on the onset of dislocation formation and its intensity at pores and hard inclusions during the deformation process. For this purpose a molecular dynamics model of an fcc metal containing pores and/or inclusions was developed. This model material was then sheared at different strain rates, thermal and hydrostatic loads and related development of the dislocation substructures investigated.

A9.10
SURFACE RELAXATIONS OF ALUMINUM SIMULATED BY BOND ORDER POTENTIALS. Shigeto R. Nishitani, Sadaichiro Ohgushi, Hirohiko Adachi, Kyoto Univ, Dept of Materials Science and Engineering, Kyoto, JAPAN; Masato Aoki, Gifu Univ, Dept of Electrical and Electronic Engineering, Gifu, JAPAN.

For the realistic simulations of the defect structures at atomistic level, reliable interatomic potentials are indispensable. However, the oscillatory damped behavior observed around lattice defects have been hardly reproduced by the simple empirical potentials. Very recently we have performed the simulations on multilayer surface relaxations of aluminum by bond order potentials with a set of transferable tight binding parameters. This novel potential successfully reproduces the oscillatory damped behavior of rough surfaces and an expansion of (111) surface. The simple model of the embedding atom methods fails the simulations of these characteristic behaviors. Further investigations on the forces reveal that the final relaxed positions can be predicted by the forces under the unrelaxed conditions.

A9.11
STRUCTURE AND BONDING OF THE RHOMBOHEDRAL TWIN INTERFACE IN α-Al_2O_3. A.G. Marinopoulos, C. Elsaesser, Max-Planck-Institut fuer Metallforschung, Stuttgart, GERMANY.

We have studied the local atomic structure and chemical bonding of the rhombohedral twin interface in α-Al_2O_3 by means of first-principles local-density functional and empirical shell-model calculations. In particular, we have considered the case where the terminating interface plane is located at vacant octahedral interstitial sites of the oxygen sublattice, in accordance with recent HRTEM observations [1,2]. These experimental observations, however, could not provide conclusive information regarding the complete interfacial structure because only images of two-dimensional projections along the $[2\bar{1}\bar{1}0]$ axis were analyzed. For the symmetrical $(01\bar{1}2)\|(01\bar{1}2)$ twin orientation the corresponding dichromatic patterns lead to a number of geometrical models for the interface, which differ from each other both in the local atomic structure and in the relative translations of the adjoining grains. The first-principles calculations yield that the structure with the lowest interfacial energy comprises a two-fold screw axis at the interface, confirming qualitatively the prediction of the empirical shell-model calculations and complementing the HRTEM observations. Furthermore, detailed insights into the local electronic structure at the interface are accessible. [1] T. Geipel et al., Acta metall. mater. 42, 1367 (1994). [2] F. R. Chen et al., Phil. Mag. A 72, 529 (1995).

A9.12
IDENTIFICATION OF 2D BOUNDARIES FROM 3D ATOM PROBE DATA, AND CORRELATION OF ATOMIC DISTRIBUTIONS WITH POSITIONS OF INTERFACES. Olof C. Hellman, Justin Vandenbrouke, Dieter Isheim, Jörg Rüsing and David N. Seidman, Dept. of Materials Science and Engineering, Evanston, IL.

Three dimensional Atom Probe microscopy produces a real space reconstruction of a majority of the atoms in samples consisting of more than a million atoms. This scale is large enough to include internal interfaces for phase separating systems or systems with small and numerous precipitates. One of our goals is to perform chemical analyses in the vicinity of these interfaces and correlate data with respect to the distance from an interface: e.g. to see how chemical distributions change in the vicinity of these interfaces. This is an example of a single analysis technique spanning from the atomic level to the microstructural level.
In this paper, we will show our algorithm for representing the position of interfaces in 3D as caclulated from Atom Probe data, which is based on methods used in computer graphics for representation of 3D objects, and we will show measured distributions of a species as a function of distance from that interface. We will also compare this method to more simple projection techniques, and show how this technique can improve the statistics of such an analysis by more than an order of magnitude. This is especially important for the case of segregation of dilute alloys, for which less than ten atoms of one species in an analysis can be considered statistically significant.

A9.13
CRACK BEHAVIOUR AT BIMATERIAL INTERFACE - A MIXED ATOMISTIC/CONTINUUM APPROACH. Arun R. Pillai, Ron Miller, University of Saskatchewan, Department of Mechanical Engineering, Saskatoon, CANADA.

Interfacial defects like grain boundaries and phase boundaries play an important role in the mechanical behaviour of engineering alloys. In particular, these interfaces can influence the fracture properties of a material. The problem of a crack on a bimaterial interface has been well studied from a continuum mechanics point of view. In this work, we study this problem at the atomic scale, with the goal of elucidating the interaction between the macroscopic elastic fields and the microscopic crack tip phenomenon. We study a bimaterial interface crack at the atomic level using the Quasicontinuum(QC) method. The QC formulation incorporates an atomistic constitutive law into a continuum finite element framework.(V B Shenoy, R Miller, E B Tadmor, D Rodney, R Phillips and M Ortiz , Journal of the Mechanics and Physics of Solids, v47(1999),p611-642). The QC method treats critical regions like the crack tip atomistically and regions away from the tip as a continuum thereby reducing the degrees of freedom and simplifying the application of boundary conditions.The underlying atomistic model used is the Embedded Atom Method.(M S Daw and M I Baskes, Phy Rev B, 29,p6443). The research has two main objectives. The first is to obtain the stress and strain fields at the atomic scale around a bimaterial crack tip and compare these with continuum mechanics predictions. The second is to study the fracture behaviour of the bimaterial crack. This behaviour is dependent on such factors as the atomic structure of the interface and the differences in elastic properties between the two materials. Our research sheds light on the importance of these factors in bimaterial interface fracture.

A9.14
EMBEDDED ATOM METHOD AND FINITE ELEMENT ANALYSIS OF ALUMINUM-SILICON INTERFACE FRACTURE. K.A. Gall, M.F. Horstemeyer, Sandia National Laboratories Livermore, CA; M.I. Baskes, Los Alamos National Laboratories Los Alamos, NM.

Fracture of silicon particles and interface debonding of the Al-Si interface has been observed during the mechanical loading of an A356 cast aluminum alloy and during the manufacturing process of interconnect lines in computers. In this study we examine the various failure mechanisms by performing Embedded Atom Method (EAM) calculations and Finite Element (FE) simulations of the Al-Si composite system. In the present study, only the [001]Si||[001]Al interface is considered. In an unloaded and relaxed state, the EAM predicts that the interface between the Al and the Si is incoherent with a mild degree of order. The study further considers the effects of applied displacement boundary conditions on the relative strength and spatial damage progression in the Al, Si, and at the Al-Si interface. The effects of boundary condition configuration, initial defect density, and atomic block size on the damage progression are studied in detail. When adjoining blocks of pristine Al and Si are subjected to tensile boundary conditions, it is demonstrated that the interface is a weak link for fracture. The interfacial failure occurs over a finite strain increment due to excessive plasticity in the Al at the micro-level. When line-vacancy defects (cracks) are introduced into the Al or Si, the failure mode (interfacial versus bulk) depends on the orientation of the interface with respect to the boundary conditions and the size of the initial defect. This work was supported Sandia National Laboratories by the U. S. DOE under contract no. DE-AC04-94AL85000.

A9.15
SELF-AFFINE MEASUREMENTS ON FRACTURE SURFACES OF PLASTIC MATERIALS BY AFM. Edgar Reyes, Carlos Guerrero, Virgilio González and Moisés Hinojosa, Doctorado en Ingeniería de Materiales, Facultad de Ingenierá Mecánica y Eléctrica, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, Nuevo León, MEXICO.

In this work, self-affinity of fracture surfaces of a semi-crystalline and an amorphous polymers were studied. Specimens of isotatic polypropylene (i-PP) and polystyrene (PS) were obtained by capillary extrusion and then immersed in liquid Nitrogen for 15 minutes. The cracking of the materials was done un heuristic conditions. The fracture surfaces generated in this way were analysed using a contact mode atomic force microscope (C-AFM). Before the measurements, the optimal operating conditions on the C-AFM were fixed. These conditions allowed us to obtain heigth profiles on several zones of the fractured samples. Using these measurements the average Hurst exponent, (H), was estimated through the variable bandwidth method. A value of H=0.788 was obtained for i-PP over two decades of length scales and H=0.805 for PS over one decade. These results are in very good agreement with the universal exponent of 0.78 reported in the literature for other materials, mainly metals and ceramics. In addition, it is proved that, choosing the adecuate operating conditions, reliable roughness measurements can be done on fracture surfaces of plastics materials using the C-AFM.

A9.16
ATOMIC SCALE SIMULATIONS OF CRACK INITIATION IN SILICON. Matti Maki-Jaskari, Kimmo Kaski, Antti Kuronen Helsinki University of Technology, Laboratory of Computational Engineering, FINLAND.

The applicability of semiempirical potential energy models for describing crack initiation and fracture in covalently bonded silicon has been studied using classical Molecular Dynamics approach. Interactions between atoms have been described with the commonly used many-body potential energy models, i.e. the Stillinger-Weber and Tersoff potentials, and the recently developed Environment Dependent Interatomic Potential (EDIP), which yield a number of structural properties of silicon correctly. The initial elastic behaviour due to these potentials are quite identical, which is no longer the case for large values of strain as indicated by large differences between the corresponding stress-strain curves. In this study we have focused our attention mostly on EDIP, but since its original form was found problematic in describing bond breaking properties we tested three different modifications of it. In addition we have studied crack tip structures observed preceding the actual fracture, by using an idealized simulations setup for a system with an initial side cut in (110) and (111) crystal plane and under tensile constant rate loading condition. Our results indicated the formation of stable ring-like structures. Unless angular forces due to the three-body term of the potential were made relatively strong, these ring-like structures were formed near the crack tip before and even during the crack initiation. These relatively stable structures could cause crack initiation to stop temporarily, especially at early stages of fracture.

A9.17
A PARTITIONED-PROBLEM APPROACH TO MICRO-STRUCTURAL MODELLING OF A GLASS-CERAMIC. Anthony C. Fischer-Cripps, CSIRO Division of Telecommunications and Industrial Physics, Sydney, AUSTRALIA.

The indentation response of a mica-containing glass-ceramic is studied. In this type of material, Hertzian cone cracks which normally occur in brittle materials loaded with a hard spherical indenter are suppressed in favour of distributed sub-surface damage indicating plastic yield. Theoretical analysis, finite-element modeling and experimental results are used to establish a connection between the macroscopic behaviour of the material and damage events occurring on the microstructural scale. This is achieved by first determining the macroscopic material properties, such as yield stress and strain-hardening index, in terms of the microstructure. These properties are then used to predict the macroscopic indentation response of the material. The problem is thus partitioned into the microstructural and macroscopic domains. This work is of particular relevance to the design of structural ceramics in machining, wear, and bearings applications.

A9.18
IN-SITU IDENTIFICATION OF MULTIPLE, SIZE DEPENDENT, PHASE TRANSFORMATIONS DURING POINT LOADING OF SILICON. A.B. Mann, T.P. Weihs, D. van Heerden, The Johns Hopkins University, Department of Materials Science & Engineering, Baltimore, MD; J.B. Pethica, Oxford University, Department of Materials, Oxford, UNITED KINGDOM.

During point-loading (nanoindentation) of silicon we used a unique combination of in situ electrical and acoustical measurements and ex situ transmission electron microscopy to identify the size dependence of pressure induced phase transformations. The transformations are found to exhibit a strong dependence on the size of the deformed volume. For all contact sizes the silicon transforms to the metallic, β-Sn phase during loading, but during unloading the final phase for nanometer size volumes is the body-centered cubic, BC8, phase while for larger volumes it is amorphous silicon. The size dependence is explained by considering how shear stress fields vary with contact size and how interfacial effects between the silicon substrate and the BC8 phase determine its stability. During the early stages of unloading of both small and large contacts the presence of a non-metallic phase (assumed to be the recently discovered rhombhedral, R8 phase) is observed. The multiple phase transformations observed experimentally are compared to quasi-continuum models of nanoindentations in silicon and the measured electrical properties are used to verify first-principles calculations for silicon's high pressure phases.

A9.19
RESIDUAL STRESSES AND CRACKING IN ALUMINA. Venkata Vedula, S. Jill Glass, Sandia National Laboratories, Albuquerque, NM.

Residual stresses arise in ceramics during processing as a result of thermal expansion anisotropy and crystallographic misorientation across the grain boundaries. The magnitude of these stresses can be

very high (200-300 MPa) and may cause spontaneous microcracking during the processing of these materials. The microstructural level stresses are likely to play a significant role in where cracks initiate and propagate under macroscopic loading too. The magnitude of residual stresses in alumina was predicted using object oriented finite element analysis and experimentally determined orientations and grain boundary energies. The crystallographic orientations and grain boundary energies were obtained by electron-backscattered diffraction (EBSD) and AFM groove measurements respectively. Crack initiation and propagation were also simulated using the Griffith fracture criterion. Indentation cracks were introduced to determine if certain boundaries were more susceptible to cracking than others. The misorientations and predicted stresses at the grain boundaries that fractured in simulations were compared to the experimental data. 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.

A9.20
DISPERSIVE MEASUREMENTS OF VELOCITY IN HETEROGENEOUS MATERIALS. M.D. Knudson, W.M. Trott, J.R. Asay, M.R. Baer, J.N. Castaneda, L.C. Chhabildas, Sandia National Laboratories, Albuquerque, NM.

An optically-recording velocity interferometer system (ORVIS) has been adapted to a line-imaging instrument capable of generating precise measurements of spatially resolved velocity variations during dynamic deformation with both high spatial resolution (few microns to few mm) and high temporal resolution (few hundred ps). The use of this diagnostic to obtain measurements of the mesoscopic scale dynamic response of shocked material has been demonstrated on several different classes of heterogeneous materials, including: foam, glass-reinforced polyester, and pressed, granular sugar (high-explosive simulant). In this presentation emphasis will be placed on the results of plate-impact, shock wave experiments performed on pressed, granular sugar in which the grain size distribution was systematically varied. Discussions will focus on (i) the data obtained, (ii) the advanced data reduction routines used to extract information concerning the mesoscopic scale processes, and (iii) critical evaluations of 3-D numerical simulations for the particular experimental configuration that incorporate physics-based models to treat the grain-boundary properties and grain-boundary interactions. The developments decribed here should provide a useful experimental/analytical methodology that can be used toward the development of better predictive, physics-based continuum models. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

A9.21
HIERARCHICAL LENGTH-SCALE INFLUENCE ON CRACK PROPAGATION IN MICROCOMPOSITES. Luke N. Brewer and Vinayak P. Dravid, Northwestern Univ., Dept of MS&E, Evanston, IL.

Fracture of materials presents a classic microstructure-property correlation problem wherein crack propagation is affected by virtually all microstructural length-scales: from intricate atomic bonding at interfaces to the macroscopic geometry of the crack trajectory to the interfaces. Fracture of ceramic micro-composites is no exception, where there are additional considerations owing to both, spatial and dimensional constraints, imposed on the individual composite phases. We have resorted to directionally solidified eutectics (DSEs) of oxide-oxide and oxide-metal materials (e.g. NiO-ZrO_2, CoO-ZrO_2, W-ZrO_2 etc..) as model microcomposite systems, where the microstructure represents either alternating single crystal lamellae or metal fibers embedded in single crystal matrix. We have conducted elaborate investigation of relevant length-scales, right from atomic structure/bonding, to macroscopic residual stresses. Crack propagation studies are conducted using both indentation-induced propagation as well as via in-situ SEM and TEM. Residual stress tensors for individual single crystal phases are measured using x-ray techniques and novel approach utilizing electron backscattered diffraction (EBSD) in SEM. Simulation of residual stresses is performed using object-oriented finite element approach which provides real-space pictorial view of 'real' microstructure of microcomposites, which facilitates correlation of crack propagation behavior with microscale residual stress distribution. A conceptual framework will be presented which takes into account the myriad of length-scale variables and the magnitude of their influence on crack propagation in DSE microcomposite systems. It will be argued that experimental techniques, especially based on electron microscopy, have advanced further enough to provide significant clues to the both the length-scale hierarchy and hierarchy of magnitude of influence from nanoscale to macroscale.

A9.22
Abstract Withdrawn.

A9.23
SELF-AFFINE ANALYSIS ON CURVED REFERENCE SURFACES: SELF-AFFINE FRACTAL CHARACTERIZATION OF TNT FRACTURE SURFACE. L.V. Meisel, R.D. Scanlon and M.A. Johnson, Benet Laboratories, US Army TACOM-ARDEC, Watervliet, NY; Y.D. Lanzerotti, US Army TACOM-ARDEC, Picatinny Arsenal NJ.

A trinitrotoluene (TNT) fracture surface image is characterized in terms of a self affine fractal structure. The fracture surface was produced by high acceleration in an ultracentrifuge when the TNT strength was exceeded. An atomic force microscope (AFM) captured the topography of a 4 μm square region on the fracture surface. The present analysis supports a self-affine fractal description of the TNT fracture surface (wavelengths of 0.016 μm to 4.0 μm) and provides a new perspective on fracture processes in TNT. An essential step in self affine fractal characterization of surfaces is the determination of reference surfaces. A self-affine fracture surface can be described in terms of a single-valued height function. In the TNT fracture surface, single-valued height functions, which describe surface texture, can only be defined with respect to curved reference surfaces. By employing curved reference surfaces, we have demonstrated that self-affine fractal scaling can be used to characterize the TNT fracture surface. This provides important information that is not evident in the analysis of individual surface scans.

A9.24
INTERFACE STRESS IN NANOCRYSTALLINE MATERIALS. R. Birringer, University of the Saarland, Dept of Physics, Saarbruecken, GERMANY.

Nanocrystalline materials are characterized by a high density of internal interfaces (grain or phase boundaries). This enables probing the interface stress by measuring the pressure exerted on the nanocrystals by the network of interfaces comprising the interfacial component of the nanocrystalline sample. For materials with fcc symmetry, we find the interface stress to be positive with a magnitude on the order of 1 J/m^2. Combining this result with measurements of the overall elastic constants of nanocrystalline materials, which can be carried out by an ultrasonic technique, we can estimate upper and lower bounds for the elastic constants of the interfaces.

A9.25
THE EFFECT OF OXIDATION ON CRACK PROPAGATION IN ALUMINUM. Timothy J. Campbell, Rajiv K. Kalia, Aiichiro Nakano, Priya Vashishta, Concurrent Computing Laboratory for Materials Simulations, Dept of Physics & Astronomy, Dept of Computer Science, Louisiana State Univ, Baton Rouge, LA; Shuji Ogata, Dept of Applied Sciences, Yamaguchi Univ, Ube, JAPAN.

Fracture of aluminum in the presence of oxygen is investigated with large-scale multiresolution molecular- dynamics simulations. The interaction scheme, which incorporates variable charge transfer among atoms, successfully describes a wide range of physical properties of Al and Al_2O_3[1]. Dependence of crack propagation on the existence of the oxide, metal-oxide interface, and the continued oxidation of fracture surfaces is presented. The effects of charge transfer, structural correlations, and stresses near the crack are analyzed.
Work supported by AFOSR, ARO, DOE, LEQSF, NASA, NSF, and USC-LSU MURI from DARPA.
[1]F. H. Streitz and J. W. Mintmire, Phys. Rev. B 50, 1199

A9.26
MICROSTRUCTURAL FAILURE MODES IN NANO-GRAIN THIN FILMS: NUMERICAL MODELS AND EXPREIMENTS. J N. Baucom, A.J. Griggs, M.A. Zikry, J. Kasichainula, North Carolina State University, Department of Mechanical and Aerospace Engineering, Raleigh, NC.

A multiple-slip dislocation-density based constitutive formulation and specialized finite-element schemes have been developed to characterize material failure on the appropriate physical scales needed for the accurate understanding and prediction of the underlying physical mechanisms that control failure initiation, growth, and coalescence in material systems of thin nano-sized ceramic films that are layered on metallic substrates. Dislocation-density transmission and blockage interfacial conditions and local stress fields have been obtained for the interface between the ceramic film and the metallic substrate. These evolving dislocation-density discontinuity conditions and local stress fields are used as failure criteria to track the initiation and evolution of failure modes such as delamination and film cracking. The interrelated effects of grain boundary orientation, dislocation pile-ups, dislocation density evolution, geometrical and thermal softening and hydrostatic stresses on failure paths and modes in these systems have

been studied. AFM and SEM studies have been used to investigate and characterize failure surface roughness and film adhesion in notched and unnotched systems. Based on the present analysis and on comparison with the AFM and SEM experimental studies and observations, it is shown delamination and film cracking can be characterized in terms of the material competition between the evolution of failure modes in both the ceramic film and the metallic substrate.