SYMPOSIUM A

Multiscale Phenomena in Materials—Experiments and Modeling

November 30 – December 2, 1999

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*Invited paper
8:15 AM #A1.1
PLASTICITY OF CRYSTALLINE MATERIALS AT SMALL LENGTH SCALES. W.D. Ng, 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 mechanical properties change significantly from nanoscale 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: (1) Dislocation Effects, (2) Microstructure Effects and (3) Stress Gradient Effects. Nanocrystalline or single-crystal samples at the nanometer scale reveal 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 are compared favorably with recent calculations of nanometer scaleindentations in perfect Au crystals. We discuss special precautions that must be taken to analyze indentation experiments at this length scale. The 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 have been 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. Macdonell, 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 microscopic plastic behavior during large deformation are analyzed in terms of tensorial property symmetry. Texture interpretations of the materials require the determination of distribution functions 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. Micromechanical crystal simulations are performed to probe a general shape for the yield surface 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 yield 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.T. Baskes, Los Alamos National Laboratory Los Alamos, NM.

Kinematic variables used for crystal plasticity and micrascle 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 plasticity and simple shear deformation were performed to discuss the various aspects of the kinematic quantities. Ties to crystal plasticity and micrascle internal state variable theory will be discussed as well.

This work was supported by 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. Bussian, 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 microscopic size of the sample (in a non-self-similar manner) and often involves pinned (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 crystal 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 an additional elastic deformation gradient field. The latter measure can play a natural role in a non-local 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 experiments. A comparison between this model and a discrete dislocation simulation is presented.

10:30 AM #A1.5
EXPERIMENTAL STUDY OF DISLOCTION VELOCITY AND MOBILE DENSITIES. Joel Beuneville, B. Le Picasso-Masterstock, 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 of mobile dislocations in the matrix 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 stress-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 dislocation storage in the crystal, this too contributes to strain-hardening. This aspect will also be considered. Recent determination of dislocation relaxation rates in two intermetallic compounds such as NiAl of the L12 structure and TiAl of the LTA 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 high for metallic glasses 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 Tatsch, Ottmar Kolodz, 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 determination, Orientation Image Microscopy (OIM) is applied to determine the crystallographic grain orientation within a selected area of approximately 200x200 um. OIM permits two thousand distinct 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 homologous points on the two photographs. Between 15,000 and 40,000 homologues points are detected within the specified area. The homologous points determine a deformation field that can be derived
numercially to obtain the local in-plane strain field. The variation of the grain orientations during each deformation step is measured by comparing the OIM phase prior and after 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 deformation gradient is used 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 Arzamendi, LPMF, Université Paris-Nord, Villetaneuse, FRANCE, Jean-L. Rapaport, 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. This may express a critical shear stress on a slip system in an sum of an effective strain depending on strain rate and temperature, and an internal 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. This is to assess, among other features of the plastic response, the importance of a local orientation distribution on the global behavior. While one rearrangement 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: SCALE-DEPENDENT ANALYSIS.
Randy B. Miller, Army Research Lab, APG, MD; Hinal Kal, UC-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 Miller et al. (1996) 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-strain 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-strain environment. To the extent that such 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 ballistically 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, Freiburg University of Mining and Technology, Freiberg, GERMANY.

Relaxation of residual stresses in metallic materials is caused by diffusion of inhomogeneously distributed solvated 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 transmission electron microscopy (TEM) investigations have been used to input data into two models (a single constitutive model by Kocks-Mecking), which describe the relaxation of tensile loading stresses. It is the aim of the magnification investigations to estimate parameters of dislocation density and mobile dislocations and to design a dislocation-related modeling using these two models. In stress relaxation tests the microstructure was connected with a rearrangement of dislocation structures and a decreasing dislocation density. The stress relaxation in 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.


SESSION A2: NONLOCAL PLASTICITY THEORY AND DISLOCATION PHENOMENA
Chair: Huijun Gao and David H. Lassila
Tuesday Afternoon, November 30, 1998
Room 208 (H)

1:30 PM A2.1
STRAIN GRADIENT EFFECTS IN BENDING. John Y. Shin, Engineering Department 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 plasticity 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 basis of scale-dependent predictions. The finite element model 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, Y. and Fleck, N.A. (1999) J. Mech. Phys. 47, 297-324. Stolken, J. S. and Evans, A. G. (1998) Acta metall. 46, 5105-5115. 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. Xu, Univ. of Illinois, Dept of Mechanical Eng, Urbana, IL; H. Gao, Stanford Univ, Div of Mechanics and Computation, Palo Alto, CA; Z. C. Xin, 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 mechanisms via a multiscale, hierarchical framework linking Taylor's dislocation hardening model to strain gradient plasticity. The motivation for developing such a theory is the 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 stress for crystalline materials and the Mises factor which calibrates the scalar measure of geometrically necessary dislocation density from macroscopic plastic strain gradients.

2:00 PM A2.3

**EFFECT ON PRECIPITATE MORPHOLOGY ON THE GRADIENT-DEPENDENT BEHAVIOUR OF TWO-PHASE SINGLE CRYSTALS.** Ethan P. Bass, Franz T. Meissner, and Noel P. O'Dowd, Department of Mechanical Engineering, Imperial College, London, UNITED KINGDOM.

During high temperature deformation of single crystal superalloys, the initial 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 mechanical-based rate and gradient dependent crystallographic formalism [1][2] is used to describe the behavior 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 mixture 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 behavior of the GND densities, and a fully implicit numerical algorithm within a large strain kinematics framework to update the total stress and internal slip system variables. Results from 3D unit cell finite element computations are compared with high resolution diffraction and selected area diffraction data and predictions of spatial gradients of local stress and internal slip system variables [3].

References:

2:15 PM A2.4


In polycrystals, localization of the plastic deformation during metal forming processes is usually considered as the root cause of large deformations and/or the result of the change of loading paths. Such heterogeneous deformation increases the ductility and leads to rupture. In order to determine, the mechanisms ruling the localization of mild steel polycrystals after change of loading paths are performed, corresponding to a plane tension followed by parallel and orthogonal uniaxial tension. The localization phenomena was analyzed on microscopic, mesoscopic and macroscopic scales thanks to different techniques such as local texture (EBSD) and microstrainometry by microgrids. SEM observations and local strain field computations pointed out that microbands of localization propagate by activation of two families of short parallel coarse slip bands. This experimental background, linked to the observations of dislocations and dislocations suggests that bifurcation is bound to the misorientation of the microstructure. By contrast, the post-bifurcation may be correlated to a textural and microstrutural 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 144 grains six times josted. The constitutive law is a viscoplastic flow 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 misorientation and evolution of the microstructure of dislocations and in other hand to get large strains and saturations of the density of dislocations. The results of the simulations are 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.** Lyde 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 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-pen 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. Myers, Cornell Theory Center, E. Miller, A. Mulfur, J. P. Selma, Laboratory of Atomic and Solid State Physics, T. J. Turner, E. Miller, P. M. Ferreira, School of Mechanical and Aerospace Engineering, S.R. Arvadhe, E. Iseul comforts, C.-S. Chen, A.R. Ingraffena, 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 analysis. Improved understanding of both statistical characteristics – such as orientation and misorientation distribution functions – and specific structural features – such as dislocation cell 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 of multiscale. We are combining techniques on several fronts to better understand the nature of polycrystalline plasticity, the formation and evolution of subgrain deformation structures, and the relationships between local orientation, misorientation, and dislocation information. 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 EBSD 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 DILOCATION MOTION IN THIN FILM SYSTEMS.** E. 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. Thomas, P.M. Ross, K. Schwoerer and M.C. Rowsell, Faraday Discussions, Royal Society 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 film 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 quantitative information about dislocation velocities, interaction stresses and...
overall strain relaxation behavior. A model materials system for studies of dislocation behavior is heterogeneous 3SiC layers grown on Si substrates, in which the difference in the 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 microcrystalline, dislocation density decreases and grows in order to relieve this mismatch strain. Quantitative observation of the interaction between moving dislocations and other interfacial misfit dislocations will be presented. These observations are amenable to direct correlation 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 the importance of phenomena of reactive blocking in heterogeneous 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 a 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 bend testing techniques, providing an important crosslink with other experimental methods of studying dislocation-based strain relaxation.

4:15 P.M.  A2.8
SURFACE FILM SOFTENING EXPERIMENTS AS INPUT FOR MODELING OF DEFORMATION AND FRACTURE
Ronak Gilani, Materials Science and Engineering, University of Michigan, Ann Arbor, MI and Sandin 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 plasticity 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 P.M.  A2.9
SIMULATION OF DISLOCATION MOTION IN CONFINED GEOMETRY UNDER NONUNIFORM STRESS FIELD
Clemmendard, DMSE, ONERA, Chastillon Cedex, FRANCE; B. Devincre, L. Kubin, LEEM, CNRS ONERA, Chastillon Cedex, FRANCE; J.L. Chatoboe, DMSE, Chastillon Cedex, FRANCE.

In order to describe the plastic behavior of crystalline materials containing structural heterogeneities and for complex loading, a new non-local model 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 mesoscale level. The basis of this new computer model is 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 P.M.  A2.10
DISLOCATION MULTIPLICATION AND STRAIN HARDENING IN BCC SINGLE CRYSTALS: 3D DISLOCATION DYNAMICS SIMULATIONS
Meijo Tang, Physics Directorate, Lawrence Livermore National Lab., Livermore, CA; Benc Devincre, Labhish P. Kubin, LEEM, CNRS ONERA, Chastillon, 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 segregation in the mobility of the screw and edge dislocations, the dislocation multiply significantly during the initial stage of 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 density and the average dislocation length, initial density, and the simulation volume size. The objective is to understand the characteristics of dislocation multiplications. The latter 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.
ranges (up to the shock stresses), for the materials with various volume fraction and impurity state, precursor strain and thermal prehistory. 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 step, the grain boundary origin, polycrystalline- nanoparticulate and amorphous state, the first microcracks nucleation, then their coalescence into microcracks (microfracture) and the formation of fracture surfaces. Structural investigations and literature data confirm that the deformation mode of the dislocation properties of dislocation double cross-slip, climb and the Orowan bowing under various types of loadings (shock, impact, Instron or creep) is the dislocation structure near the fracture tips, the corresponding fracture modes (so called ductile, brittle or cleavage one) and the structures of rupture surfaces differ to a great extent from each other. [1] V.P. Kiel, Mser. Sci. Engr., 1993, 164 A, 356. [2] V.P. Kiel, Proc. of ISMA-9, Hau, 1, 601 (1991).

A3.4 SURFACE INSTABILITIES AND PLASTIC DEFORMATION OF COPPER/TANTALUM CYLINDRICAL CONDUCTORS. J. Colin, J. Grillet, Université de Poitiers, Laboratoire de Metallurgie Physique, SP2MI Futurescope, FRANCE; L. Thilly, F. Lecouturier, S. Akselnyi, Service National des Champs Magnetiques Puissants, CNRS UPS INSa Toulouse, FRANCE; J.P. Peyrade, Laboratoire de Physique de la Matière Condensée, CNRS UPS INSa, Toulouse, FRANCE.

When a solid is submitted to non-hydrostatic stresses, sinusoidal fluctuations can develop and grow by diffusion to release the stored elastic energy; this is the Anser-Tiller-Grillet instabilities. The formulation of Anser-Tiller-Grillet instabilities has been modified to model the dislocation of two sets of surface instabilities which have been observed on the relaxation of more than a month in cylindrical conductors under stress. Axial and radial sinusoidal fluctuations have been introduced simultaneously on the cylindrical shape of a stressed conductor. The stress relaxation has been calculated and an energy variation has been performed to determine the threshold wavelengths of these oscillations. A study of the cylinder surface kinetics has been performed to characterize the evolution of the roughness versus time. The different effects 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. Xinghong 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 AlAlxx and AlxxAl aluminum sheet metal alloys. A dislocation-based viscoplastic model is formulated for the interaction of the dislocation configurations 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 AlAlxx and AlxxAl aluminum alloys.

A3.6 A MODEL FOR CALCULATING SUBSTRATE CURVATURE DURING COALESCEANCE 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 TEM reveals microstructural characteristic 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 Å, followed by a change towards a tensile maximum at 30 Å, after which the stress becomes compressive again. Plan view TEM of Pt films of thicknesses ranging from 3 Å to 35 Å 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 dislocations and islands are seen as 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 ZrC2-Based Laves Phases. Won-Yong Kim, David E. Laughlin, 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 applications 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 dramatic 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 ZrC2-phased alloy system was conducted and is reported here. Compression tests were carried out on ternary Zr-C-X(X = He, H, 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 Muto, Hokkaido University, Institute 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 didn't 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 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 reflection microscopy 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. Through, 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 Guichard, O. (1996) Crack velocities in freshwater and saline ice. J. Geophysical Research., 101(B5): 11541. 2. Arakawa, M., Petrenko, V.F. and Muto, N. (1998) Propagation of cracks in ice with liquid inclusions. Proc. of the 1998 Annual Meeting of Japanese Society of Snow and Ice, p. 41.

A3.9 STRESS AND TEMPERATURE DEPENDENCE OF Gn PENETRATION RATES IN A HIGH STRENGTH Al ALLLOY. Boxiong Ding, Richard G. Hoggland, 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 have 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 N00014-97-1-0897.

A3.10 CRITICAL GROWTH OF FRACTAL FATIGUE DEFECTS

Material defects growing during fatigue or damage process are described by fractal defects. The realistic effect on the fracture toughness 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 irreversable process are determined by characteristic (for a given material) fractal measures. The defects localization runs in accordance with characteristic measures and remains proportional for finite characteristic measures. The microscopic range of length scales has been introduced via additional dependence upon microscopic volume limiting defects evolution. The involved parameter determines the Haasdonk distance from defects structure to the microscopic range of scale. 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 microscopic limits 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 length. The singularity appears at a solution 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) microscopic 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 characteristic measures as well as the irreversible fatigue evolution threshold.

A3.11 LONG DISTANCE FRACTURE SURFACE ROUGHNESS ON A DENDRITIC ALUMINUM ALLOY. J. Alback, F.-J. Geza, M. Hinojosa, Facultad de Ingenieria Mecanica y Electronica, 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 Forced Microscopy SEM and stylus profilometry allowed us to cover a wide spectrum of length scales, spanning from a few nanometers 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 TIN FILMS. Erica T. Lilleodden, William D. Nie, Stanford University, Dept of Materials Science & Engineering, Stanford, CA.

Indentation is an obvious experimental technique for exploring the predictions of multiscale 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 at the initial stages of indentation imply that dislocation nucleation occurs. Atomistic simulations of idealized indentation configurations have shown that surface nucleation of dislocation loops occurs at near-theoretical shear stresses. Such studies have provided a basis for correlation of experimental observations, but simulations of realistic indentations are not yet available. Experimental observations of discretized indentation behavior in Cu oriented films will be described in terms of both dislocation modeling and strain gradient plasticity. FE simulations have been used to extract the effective yield strength 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 accounting for plastic work. The discrepancy equation is expressed in terms of a constant contact area during indentation emission. Additionally, it is shown that the observed hardness-displacement relationships deviate from the strain gradient model prediction due to dislocation deformation which dominates 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 Vaclav V. Bata, 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 and/or local scales, plastic deformation is modeled at different structural levels, from a small volume of single crystal to the aggregate response of individual slip/twin systems. 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-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 possible mechanisms of deformation in polycrystals, including grain boundary irregularities, twist energy, and inter-grain sliding.

A3.14 THE DETERMINATION OF EVOLVING MICROSTRUCTURE USING CONSTITUTIVE RELATIONSHIPS. Brad J. Disk, Peter Porubka, Shig Shimoto, 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 evolution using electron microscopy and Raman spectroscopy. From such studies considerable understanding of the origin of flow stress has been delineated but it's evolution to the measured stress-strain curve has been almost ignored. Our studies using high resolution load-indentation data show that the mean slip distance, \( \lambda \approx 0.5 \pi \frac{SG}{\tau} \) is functionally correct but the absolute correct value is too high even at low temperatures where dynamic thermal recovery is negligible. The earlier work on dynamic sensitivity measurement indicates that mechanical sensitisation is possible even during Stage II suggesting a quantifiable relation between \( \lambda \) and \( \phi_r \) which will result in a suitable proportionality factor. To examine the basis of this hypothesis, uniaxial tensile tests on nearly random oriented pure AI specimens of ultra-fine grain size (2-4 \( \mu \m \)) were performed at various sub-ambient temperatures. The fine grain size which is stable at 230°C for 100 hrs. was a upper limit to \( \phi_r \). By plotting \( \lambda \) versus flow stress, a minimum is observed which correlates well with published deformed cell size in a function of stage II. From such studies considerable understanding of the origin of flow stress has been delineated but it's evolution to the measured stress-strain curve has been almost ignored. Our studies using high resolution load-indentation data show that the mean slip distance, \( \lambda \approx 0.5 \pi \frac{SG}{\tau} \) is functionally correct but the absolute correct value is too high even at low temperatures where dynamic thermal recovery is negligible. The earlier work on dynamic sensitivity measurement indicates that mechanical sensitisation is possible even during Stage II suggesting a quantifiable relation between \( \lambda \) and \( \phi_r \) which will result in a suitable proportionality factor. To examine the basis of this hypothesis, uniaxial tensile tests on nearly random oriented pure AI specimens of ultra-fine grain size (2-4 \( \mu \m \)) were performed at various sub-ambient temperatures. The fine grain size which is stable at 230°C for 100 hrs. was a upper limit to \( \phi_r \). By plotting \( \lambda \) versus flow stress, a minimum is observed which correlates well with published deformed cell size in a function of stage II.

A3.15 Abstract Withdrawn.
SESSION A4: DISLOCATION DYNAMICS – EXPERIMENTS AND SIMULATIONS
Wednesday, December 1, 1999
Room 208 (H)

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

The first 3D Discrete Dislocation Dynamics code was initiated by Rubin, Brachet and Camou 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 memorized 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 L12 alloys (Devreese et al., 1997), to compute parameters involved in macroscopic behavior laws (Thibault et al., 1997), and to simulate the nanocrystallization test (Fivel and Robertson, 1998). Specific versions of the code have also been developed in order to deal with other crystallographic structures such as cubic (Moulin et al., 1997 on silicon) and h.c.c. (Tang et al., 1998 on tantalum). All those codes can be seen as powerful tools which fills the gap between atomistic 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

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 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 traveled 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 pile mechanism. The nature of these tangled 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 results are unique observations of dislocation generation and motion can 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 *A4.3
DISLOCATION DYNAMICS OF PLASTIC DEFORMATION IN MOLYBDENUM. Mario Born, Vasily Bulatov and Tong-Kea Liu, Lawrence Livermore National Laboratory, Livermore, CA.

Early stages of plastic deformation and the underlying dislocation behavior in Mo are examined using off-ID-1D algorithms. Initial dislocation arrangements were generated to mimic realistic TEM dislocation microstructures in the annealed Mo single crystal. The simulated deformation response indicates the onset of plastic yield and the development of characteristic cross-grid patterns dominated by the screw dislocations. Although the initial microstructure has no dislocation sources, multiplication occurs naturally as the pinning points formed by core-climbing and vacancy superslips 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 *A4.4

We present Molecular Dynamics and Quasicontinuum simulations of 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 into Dislocation Dynamics codes to simulate irradiation hardening at the micro-scale.

10:45 AM *A4.5
DISLOCATION FOREST INTERACTIONS: SIMULATION AND PREDICTION. L.K. Wickham, 1 K.W. Schwartz, 2 J.S. Solcien. 1Lawrence Livermore National Laboratory, Livermore, CA; 2IBM 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: isochronal simulations of a dislocation and an interstitial in a dislocation are consistent with the prediction from a dislocation and an interstitial in the structure under stress. The resulting crosstalk” state provides an additional type of connection between dislocations. We present results on the persistence of junctions and croslinked 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 *A4.6
MODELING FOREST HARDENING AND DISLOCATION PATTERNING WITH A 2D SIMULATION. D. Gomez-Guzman, B. Devreese and L. Kubin, LEM, CNRS-ONERA, Chatillon Cedex, FRANCE.

Based on the results of 3D simulations of dislocation dynamics in pure metals, a simplified 2D model for multiphase has been designed. This computer model quantitatively accounts for all dislocation properties like source multiplication, sessile junctions and cross-slip. Special attention was paid to the question of glissile interstitial clusters at the boundaries of the simulation box. The results are found to correctly reproduce a linear increase of the 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 ATOMICISTIC THEORY TO EXPERIMENTS. Vasily V. Bulatov, Lawrence Livermore National Laboratory, Livermore, CA.

Dislocation motion is known to control crystal plasticity under stress. Naturally, the mechanism of dislocation mobility commanded much attention in the past and remains 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
SESSION A5: DISLOCATION CORE PROPERTIES AND EFFECTS

Chairs: Vasiliy V. Bulovic 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 atomic 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$_3$Al, the mesoatomic powder flow properties of NiAl and the deformation of gamma-$\gamma'$ at higher temperatures.

2:00 PM A5.2 PROPERTIES OF THE DEFORMATION MICROSTRUCTURE IN Al-RICH GAMMA-TIALI DEFORMED BY ORDINARY DISLOCATIONS. Fabienne Gregor, LPMT, Université Paris-Nord, Villetaneuse, FRANCE, Patrick Veyssiére, LEM, CNRS-ONERA, Chatillon, FRANCE.

In the near vicinity of the $<111>$ orientation, gamma-TiAl deforms via ordinary $1/2<110>$ dislocations. As for deformation by $<111>$ dislocations, the flow stress shows a peak at about 600°C. We present the result of an extensive microstructural investigation aimed at identifying the mechanisms 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 segmentations become gradually more pronounced with increasing deformation temperature. This effect is accompanied by a strong tendency towards cusp formation. It is found that the immobilization along the screw direction takes place prior to dislocation pinning. In addition, dislocation core 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 ATOMIC 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 neutron elasticity theory. On the atomic 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 anomalously materials.


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 parameterized tight-binding method and the energy consists of the bond part that comprises contributions from electrons, the central-force many-body part that reflects the environmental dependence of overlap repulsion arising from the valence electrons and a repulsive pairwise 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 the mechanical behavior of the 4d and 5d transition metals. These results were supported in part by the Advanced Strategic Computing Initiative of the U.S. Department of Energy through LLNL, grant no. 831542 (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 a abrupt change in the variation of the critical reached shear stress, $\tau$, with temperature, $T$. This implies a change in the deformation mechanism at a critical temperature $T_c$. In the experiments examined so far in our laboratory and elsewhere, this critical temperature appears to coincide with the brittle-to-ductile transition temperature, $T_{BDT}$. 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 characteristics induced dislocations below and above $T_c$ 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-to-ductile transition in these materials has been proposed.

3:30 PM A5.6 ANGULAR SCALE SIMULATIONS OF SCREW DISLOCATION CROSS SLIP IN Cu. T. Vegge,1, O.B. Pedersen,2, T. Leffers2, and K.W. Jacobsen1; 1Center for Atomic-Scale Materials Physics (CAMP) and Dept of Physics, Technical Uni of Denmark, Lyngby. DENMARK, 2Riso Nat Lab, Roskilde, DENMARK.

Cross slip of screw dislocations is a fundamental process in plastic deformation, where it is involved in both the multiplication and annihilation of dislocations. The phenomenon 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 stress and energy 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-constrcted 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. Perandi*, M. Robles and K.
DIFFERENT RELAXATION MODES OF EPITAXIAL AuNi ALLOYS.

Jany Thibault, Cyril Dressler, Pascale Baille-Guillermud, CEA/DRFMC/SP2M, Grenoble, FRANCE.

It will be shown that the mechanism that takes place at a nanoscale 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 an Au$_{75.5}$Ni$_{24.5}$ alloy which is representative of all the other materials in the family and with a large miscibility gap. The structure and the stability of Au$_{75.5}$Ni$_{24.5}$ 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 may play a role. Furthermore different mechanisms can occur successively. Mixing at the interface, twinning, phase transformation have been seen with the stress. The evolution of the Au$_{75.5}$Ni$_{24.5}$ alloys with temperature has also been 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 relieves the stress. It is noticeable that atomistic simulations including disclivities from this work predict the same behaviour. The alloy evolution has also 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, 1989
8:00 P.M.
Exhibition Hall D (I)

A6.1
A TEM STUDY ON THE DYNAMIC PROPERTIES OF DISLOCATIONS IN BCC METALS.
Luke M. Huang, Lawrence Livermore National Laboratory, Materials and 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 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 in BCC metals. The dislocation dynamic structures (dislocation density, configuration, free dislocation line, kink and jog on dislocation line) can affect all the aspects of dislocation properties during plastic deformation. The dislocation structures and configurations as well as the dislocation structures after quasistatic compression and shock deformation are studied and compared. Emphasis is placed on the dislocation multiplication and the dynamic motion of dislocations. The results of experiments of grid-screw, grid-nick, grid-dipole, grid-jog, grid-line and grid-dislocation will be discussed and reviewed.

A6.2
AB INITIO STUDY OF DISLOCATIONS IN MOLECULAR CRYSTALS.
Maja M. Kokot, A. Barry Kurt, 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 cyclohexane trinitramine (m 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 [011] 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 conduction band whereas these states deep within the band gap. This contributes strongly to properties of the RDX crystals creating favorable conditions for the N-O2 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 in RDX is proposed. An illuminated system of self-consistent 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 380 are core electrons. A split valence basis set as used here consists of 1470 basis functions. A single HF calculation with CRYSTAL.09 on a Multiport SUN Enterprise 4000 system with 12 Ultra Spur II processors (250MHz) in a parallel version with four processors runs for 2 days demanding significant resources of the 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 of propagating through the crystal stimulate a further dramatic gap reduction increasing the probability of electron excitation. This, in turn causes molecular dissociation via an excitonic mechanism and to start a chain reaction and explosion.


This work continues earlier efforts to understand the yield stress anomaly in LiF alloys using computer simulations of dislocation motion. The elastic self-interaction of dislocations are taken account within an isotropic approximation and simple rules are used to account for the cross-slip process in the 3D geometry of the nanocrystalline polycrystal. The simulations are carried out for a choice of parameters appropriate for the yield strength anomaly in NaI. It is found that dislocation velocities are a nonlinear function of stress. At high stresses, dislocation selfimmobilization rapidly as low stress results in high dislocation velocities. 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 Migeul, A. Vespignani, The Abuds Salam International Centre for Theoretical Physics, Trieste, ITALY, S. Zapperi, PMMI-ESPCI, Paris, FRANCE.

The viscous 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 amusingly rich but poorly understood process. 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]. Studies of changes of individual 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 breaking of a pile of these defects. The AE experiments, however, have only indirectly demonstrated part of 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 a 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 provide this picture together with a test of the predictions of the model. Furthermore, we show that the results of our simulations are dependent on the particle density in the system of dislocations. Finally, we demonstrate that the results of the present simulations depend on the particle density in the system of dislocations, as well as the possibility of mutual annihilation of these line defects characterized by its Burgers vector.

A6.5 NUCLEATION, BLUNITING OIL PROPAGATION OF A NUCLEATION, BLUNITING OIL PROPAGATION OF NANOCRACKS IN FIELD ZONES OF BNN CRYSTALS, Q.Z. Chen, W.Y. Chi, K.W. Guo, B. Gu and Y. Zhang, Department of Materials Science, University of Science and Technology Beijing, Beijing, CHINA.

Nucleation, blunting and propagation of nanocracks in dislocation-free zones (DFZ) ahead of crack tips in ductile and brittle metals have been investigated by tensioning in situ with a TEM, and analysed using microstructure mechanics. The results show that in either ductile or brittle metals, many dislocations could be emitted from a lowed 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 as a cleavage microcrack rather than being blunted.

A6.6 THE ENERGY OF DISLOCATION-OBSTACLE INTERACTION BY 3-D QUASICONTINUUM SIMULATIONS, Koeing Healy and Rob Phillips, Div. of Engineering, Brown Univ., Providence, RI.

A recently developed method to incorporate periodic boundary conditions in three dimensional quasicontinuum simulations used in study of interactions between dislocations and 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 ALCHIGA-TAI SINGLE CRYSTALS DEFORMED DETERMINATION BY DISLOCATIONS OVER THE DOMAIN OF FLOW STRESS ANOMALY, Fabienne Gregori, LPM/TM Universite Paris-Nord, Villeneuve-Saint-Georges, FRANCE; Patrick Veysseyre, LPM CNRS-ONERA Chatillon, FRANCE.

Itchigga TaI single crystals deform essentially by motion of <111> 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 dislocation mode of <111> dislocations in their slip plane, (iii) the locking properties of <111> 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. Chronis, Dept of Materials Science and 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, cyclically driven, Frank-Read source. The dislocation is treated as a linear mass and is assumed to be a linear spring between the dislocation and the surrounding medium. Energy losses are calculated for driving frequencies in the range from 1 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 theories for unbounded 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 Delbôeuf, Jaime Marín, Joaquin Lodi, DENIM, Universidad Politécnica de Madrid, Madrid, SPAIN; Tomás Díez 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 content of Cu in steels, Cu precipitates from inside the γ-Fe surrounding matrix and considerably contribute to the hardening of
the material through dislocation interactions. The neutron damage associated with these particular conditions and the formation and evolution of defects have not been well understood. Also, the processes and effects related to these mechanisms are not directly observable by my experimental means so a computer simulation methodology based on Molecular Dynamics and Kinetic Monte Carlo has been used to approach the study of a Fe-Cu alloy. The study has been made using the MDCAST code in which the Addack (Finnis-Sinclair) many-body potential has been implemented. At DENH 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. As formation, binding and migration energies corresponding to different Fe-Cu defect structures have been calculated. The 0.6 eV and 6.9 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 other dislocations while Cu interstitials seem to be less mobile than Fe interstitials in the same conditions. Finally, a probable Cu precipitation tendency has been observed in our KMC simulations.

A6.10
**OPTIMIZED SIMULATION OF DISLOCATION DYNAMICS:**
**METHOD AND VALIDATION TESTS.** R. Maier, B. Devincenre and L. Kabin, Laboratoire d’Etudes des Microstructures, CNRS/ONERA, Chassieu, 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 simple description of the properties with 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 conditions. 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 expected. First, its CPU requirement increases extremely fast with increasing number of segments. Hence, computations are restricted to small samples (≈ 3500μm) and small plastic strains (≈ 1%). Secondly, the simplicity of the edge-screw line model used to discretize dislocation curvature makes the calculation of the elastic properties less accurate. Due to 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. New, additional slip systems were 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 as 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 evolution under plastic deformation of metallic material up to large strains and the coupling between microstructure and mechanical behavior can be modeled 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 dislocation 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 microstructure 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 Shimoto, Hiao Jin, Ke Zhang, Peter Perzako, Dept. Materials & Metallurgical Engineering, Queen's University, Kingston, Ontario, CANADA.

In the phenomenon of phasic deformation, the precise role of the internal stress process is currently evolving and many hardening mechanisms remain still not well understood and leads to ambiguities in the qualitative analysis of thermally activated flow. The composite work hardening theory of Maghribi predicts that the internal stress in the tangled walls are opposite in sign to that in the cells. However, the flow stress is not a function of detecting the complex cellular effect. The measured work done 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 gecering specific solution, results in a specific structure with 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 & & , does not increase to that of the residual stresses. 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 the recrystallization and deformation the residual stresses arise due to strain compatibility among the grains, of the order of less than 0.001%, and decrease to zero only after a discontinuous large grain growth. The flow stress is due to the dipole dislocation density in the tangled walls.

A6.13
**MULTISCALE MODELING OF ELECTROMECHANICALLY-DRIVEN VOID DYNAMICS AND FAILURE IN METALLIC THIN FILMS.** M. Rauf Ganger and Dimitrios Mardas, 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 film structures. The failure is driven by transgranular void dynamics and interface intergranular void evolution under stress. Our multiscale 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 of the void 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 misorientation 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 void propagation, while the second is stress-driven and leads to formation of convex 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 film. Furthermore, we demonstrate that the range of morphological stability depends strongly on the misorientation 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 using the micro-twist and surface electromigration using an embedded-atom-method parameterization 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 multiscale modeling framework.

A6.14
**MECHANICAL LOSS ASSOCIATED WITH STRESS ANOMALY IN Ni50Al50 and Ni50Al50 [A1(Ta)] SINGLE CRYSTALS.** E. Caprino, M. Böcking, B. Cheng, M. Demura, R. Schäfler, N. Baba and J. Bonseville, 1 Ecole Polytechnique Fédérale de Lausanne, Institut de Génie Atomique, Lausanne, SWITZERLAND, 2National Research Institute for Metals, Mechanical Properties Division, Tsukuba, JAPAN.

Dislocation dynamics in Ni50Al50 and Ni50Al50 [A1(Ta)] single crystals has been investigated by measuring mechanical loss and shear moduli as a function of temperature in the range 100 K - 1200 K. Measurements were performed in free and forced torsion pendulum. 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 assigned to the stress re-orientation of defects heated 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 conditions, i.e. the 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 percent. This maximum completely vanishes at 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 cooling. This behavior is discussed in terms of pinning of screw dislocation segments via cross-slip from the (111) onto the (100) planes (Koss-Wilford lock). After extraction 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 (100) cube planes.

A6.15
MOTION ANALYSIS NEAR SURFACE PLASTIC DEFORATION INDUCED BY THERMO-MECHANICAL FATIGUE ON 316L STAINLESS STEEL PART 1/2
EXPERIMENT S. Christine F. Robertson, S. Poissonet, A. Fiasco, 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 x 20 x 20µm), located close to the surface. This deficiency is necessary for which electron transmission 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 50µm deep indenters are performed on 3 millimetre 316L steel disk samples. Next, the samples are cyclically heated up and cooled down at a rate of 0.2°C/min [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 disk using back side electro-polishing technique [6]. A comprehensive analysis of the TEM observations has been facilitated by detailed results from numerical simulations of the performed tests [see part 2/2].


A6.16
MOTION ANALYSIS NEAR SURFACE PLASTIC DEFORATION INDUCED BY THERMO-MECHANICAL FATIGUE ON 316L STAINLESS STEEL PART 1/2

A6.17
SIMULATION OF EQUILIBRIUM DISTRIBUTION OF DISLOCATIONS IN BCC SINGLE CRYSTALS UNDER CYCLIC LOADING
S. di Niro and J.H. Morris, Ames Laboratory, Iowa State University, Ames, IA.

We are investigating the collective motion of large number of dislocation network in bcc single crystals under cyclic loading using a numerical method that describes the finite element method and multipole 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 dislocation network 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 model. The evolution of dislocation segments Branching 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. Khantia 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 the presence of a high temperature for example for a crystalline oxide. This effect is due to the low temperature of the crystalline oxide. The opening of a crack in the brittle-ductile transition. We present a model for the dependence of the critical temperature on the rate of loading and evaluate its relevance to the strain-rate dependence of the brittle-ductile transition.

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A6.19
STUDY OF ELECTRICAL PROPERTIES OF DISLOCATIONS IN ZnSe AND ZnS USING ELECTRIC FORCE MICROSCOPY
Victor P. Petrovsky, Guangfeng Hui, 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 photoc conductivity of these materials. Undoped single crystals of ZnSe and ZnS with specific microstructure were used. EFM was performed to study the dependence of electric charge of dislocations induced in the crystal 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 dislocations, screw, edge, 60°-degree) was determined by measuring surface topography in intermittent mode of SPM [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 photoc conductivity of ZnSe and ZnS. For that purpose we injected 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 dislocations are then compared with theoretical calculations. 1. O. Yu. Nikolaevsky and V. P. Feretov, Study of dislocations in ZnS and ZnSe by scanning force microscopy, 1994. J. Vac. Sci. and Technol., 12 [4], p. 2443.
A6.21 EVALUATION OF THE CONSTANT LINE TENSION APPROXIMATION IN AN ATOMIC CONTEXT.
David L. Obreja, Rob Phillips, Brown Univ, Div of Engineering, Providence, RI.

In practice, much of the work using dislocations to investigate or explain metallic 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 atomic 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 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 POSITIONAL ANNihilation METHOD. Adrian A. Panaev, and M. Kornihov, Institute of Electronics, Dept. of Position Diagnostic, Tashkent, Uzbekistan.

The modern methods of the microstructure control must 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-position annihilation (EPA) data for plastically deformed stainless steels 10X18H10T and compared with AISI 316 (Fe 65%, Cr 18%, Ni 11.5%, Mo 1.5%, Si 1%, C 0.3%). The angular distributions of annihilation photons (ADAF) of a stainless steel specimens in an interval of a strain from 2 to 20% are measured. It is shown that the half-width of a CAF curve monotonically decreases with magnification of a degree of a strain. Three stage of plastic deformation from EPA data is established. In the strain obtained by a method are indicated and are compared to data obtained by a method of acoustic emission (AE).

<table>
<thead>
<tr>
<th>Method</th>
<th>1 stage</th>
<th>2 stages</th>
<th>3 stages</th>
<th>4 stages</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>0.2 - 2.2 %</td>
<td>2.2 - 10.2 %</td>
<td>10.2 - 28 %</td>
<td>&gt; 30 %</td>
</tr>
<tr>
<td>EP</td>
<td>0 - 3.5 %</td>
<td>3.5 - 10.5 %</td>
<td>10.5 - 19 %</td>
<td></td>
</tr>
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</table>

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 determined mainly. The further growth of a strain of a simple results to increasing of concentration of defects and overwhelming number of positions are captured on defects. Is shown, that on the second stage of plastic deformation practically all positions annihilate from the capture of the dislocations (the parameters leave on saturation). From experimental spectra the concentration of dislocations for wide varieties of degrees of a strain are designed. The further development of a strain results in formation of complexes of vacancies and microcubes (third stage of plastic deformation). For want of it the parameters become insensitive to micropits with sizes more 50. Further magnification of voltage (more than 30%) 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.

2. V. V. Korjekov, L. P. Melitinskii. Fizika Metallov i Metallovedenie 58, (1964) 486.


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 properties 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 approximate 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 approximate 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 a 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 and crystal of lower symmetry by the same reasoning. The approach provides a technique for calculating elastic constants of single crystals of intermetallic at temperatures and compositions where experimental determination is difficult or infeasible.

A6.24 ON THE INTERACTION BETWEEN POINT DEFECTS AND DISLOCATIONS. Cyril R. Puc, Remaxler 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 coupling 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 Peierls stress of the dislocation than that which stood out of it. Attention is focused 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 is presented.

A6.25 DIFFUSION MOBILITY IN TWO-DIMENSIONAL LENNARD-JONES MATERIAL. Nicholas Buiy, Jeffrey Tomasi, James Sehan, Physics Dept, Cornell Univ, Ithaca, NY; Christopher Myer, 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 work will be used as input parameters in larger scale simulations involving many defects. We present atomistic simulations of defect motion in a two-dimensional material consisting of atoms interacting through a model 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 is hysteretic or continuous, i.e. first or second order. Before the barrier 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 above 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 subjected to Lennard-Jones damping forces. Conditions were chosen so that the dominant phonon modes are damped as completely as possible.

A6.20
JOINING OF ATOMIC TREATMENT AND ELASTIC CONTINUUM TREATMENT IN EDGE DISLOCATIONS.
Masao Dozuma, Y. Kogure, Tokyo University of Science and Technology, Ueno-hara, Yamamato, 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 \( r_s \). This part is referred to as the dislocation core, and the linear elastic theory is said to break down in this region. The integrals which are involved in calculations of dislocation energy use \( r_s \) as a lower limit of the radius. This procedure is unsatisfactory in that without knowing the exact arrangements of atoms in the core, it is necessary to have a value of \( r_s \) which has 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 dynamics using embedded atom potentials. The results are compared with those obtained 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 theory, 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.L. McManus, J. N. Gorman and R. C. Freeman, Northwestern University, Evanston, IL.
Reliable dislocation properties theory for metals, and especially for intermetallics, remains a challenge since an accurate microscopic description of interatomic 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 combination of the modified Peierls-Nabarro model with discrete representation of dislocation stress energy calculated by ab-initio techniques. This scheme reveals new capabilities of the PN model concept for understanding fundamental features of dislocation behavior and their characteristics in intermetallics and multiple complex stresses. 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 interatomic interactions (\( \gamma \)-surface geometry and chemical bonding).
All this is illustrated with realistic examples for dislocations in pure metals (Au, Ir, Al) and intermetallic compounds Li\textsubscript{2}Ta\textsubscript{4} and Cu\textsubscript{2}NiAl with \( \gamma \)-surfaces calculated using \( \alpha \)-initio methods. We find that in agreement with experiment the unite dislocation in Ta\textsubscript{2} is compact and split Peierls stress is equal. The calculated dislocation structures are in good agreement with available electron microscopy measurements. The experimentally observed hierarchy of slip modes, low temperature deformation behavior and TEM measurements in [101] direction are explained. In particular results show that a small elastic anisotropy and alloying effects determine observed relation between Peierls stress for edge and screw orientations. Thus, method allow to modify traditional views on dislocation core structure evolution in the process of dislocation motion and for with external stress.

A6.28
QUANTUM TUNNELING OF DISLOCATION KINKS IN COPPER.
Saw-Aun Cheong and James P. Sethna, Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY; Toya 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. As a function of temperature, time and atmospheric pressure, two different dephasing effects related to symmetric tunneling states have been observed in Cu, Ti, and Fe\textsubscript{3}B\textsubscript{20}, and are sensitive to the deformation history. Ghosy behavior in the response of heavily dislocated aluminum has been attributed to quantum tunneling centers. Quantum dephasing of conductor electrons in metads at low temperatures has recently been associated to scattering from tunneling systems. Kinks on dislocation lines are excellent candidates for these tunneling centers: they are naturally symmetric, and the small effective barrier height of the extended core structure of the defect spreads the momentum 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 Prato, L. Lizzurrini, Giancarlo Salvini, CNR-MAFEI, Pisa, ITALY; Marco Natali, Marina Berti, Davide De Salvador, Antonio V. Drago, INFM, Physics Dept., University of Pisa, Pisa, ITALY; Giacomo Torno, Gilberto Rossotto, CNR-LICHTIMA 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 characterization of the defects in tensile and compressive MO-CVD grown InGaAs/InP layers. A large number of samples has been grown and characterized by HREM, 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 2400um. In compressive InGaAs/InP layers strain relaxation is found to follow the same curve previously reported for MBE-grown InGaAs/InP 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 symmetric with the preferential relaxation covering 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 mismatch and on the [110] in-plane direction. Strain relaxation at low misfit is governed by the formation of 60 \( \cap \)\( \bar{c} \)\( \cap \) 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. Groves form in 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. Maja M. Kudija, Electrical Engineering Department, University of Wisconsin, Madison, WI, Institute of Chemistry, University of Ljubljana, Ljubljana, SLOVIA.
Yttrium Aluminum compounds are important materials, which technological applications range from lasers to propulsion systems. For example, the Nd\textsuperscript{3+} doped YAG is a well-known laser material whereas YAG:Al\textsubscript{3}O\textsubscript{2} is found to be an ideal material for high-temperature ceramic applications. In the present study, theoretical predictions of defect properties in Yttrium-Aluminum Perovskite (YAI\textsubscript{3}O\textsubscript{5}) and Garnet (\( Y_3\text{Al}_5\text{O}_{12} \)) crystals were performed in terms of two-electron potentials coupled with the classical shell model description of the point defects. A set of parameters for the lattice structure was tuned to allow model atomic structures of different types of the intrinsic (vacancies, interstitials, antisites) and impurity (\( \text{Cu}^{+}\), \( \text{Mg}^{2+}\), \( \text{Ba}^{2+}\), \( \text{Sr}^{2+}\), \( \text{Cl}^{-}\), \( \text{Fe}^{2+}\), \( \text{Ni}^{2+}\), \( \text{S}^{2+}\) ) 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 both compounds the antisite disorder is more favorably placed than the Shockley-like dislocation. It is shown that rare-earth substitution \( Y_3\text{Al}_5\text{O}_{12} \) 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.
\section*{A6.32 \textbf{MICROSTRUCTURAL MECHANICAL PROPERTIES ON A NANOVERTEX SCALE - NANOINDENTATION EXPERIMENTS AND FINITE ELEMENT SIMULATIONS.} Mahindan Pillai, 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 in the range of 100 nm are observed, to optimize the macroscopic strength and fracture resistance. Simulations of the microstructural material behavior require knowledge of the material parameters on the length scale of these small microstructures. Nucleation models for the formation of small precipitates now allow 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 structures are never observed. Results of microstructural evaluations of TiAl alloys and small precipitated phases (intermetallic compounds) are presented. AFM images of impressions left by nanoindentations often show microstructural 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. Hysteresis stresses can be extracted from load-displacement curves, by comparing them with simulations. Finite element simulation can be performed, where a small precipitate is embedded in a matrix of different materials. With these simulations, the influence of the microstructure on experimental measurements could be determined, and accuracy limits of the nanoindentation method were obtained.

\section*{A6.33 \textbf{ATOMIC SIMULATION AND EXPERIMENTAL INVESTIGATION OF ULTRA PRECISION CUTTING PROCESSES.} Ruediger G. Rentsch, Laboratory for Precision Machining (LPM), 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 workpiece layers require an effective process 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 is 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 verification of the MD models provide a basis for the extension of the model of cutting processes into the atomic range. Beyond common deformation and structure analysis, extended analysis allow for examination of the atomistic temperature and pressure 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 rate, and deformation conditions. Such simulation is useful in particular for the calculation 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.
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 interaction, boundary conditions, and 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. Nicole Blanch and Rob Phillips, Division of Engineering, Brown University. Ron H. Miller, Department of Mechanical Engineering, University of Saskatchewan, CANADA.

The quasicontinuum method is a finite element based mixed atomic-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 Brown lattice with a basis. In these materials, coherently uniform strains 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 in fracture in Zr and Nb-based ordered alloys. Zr has been known to undergo bcc to (simple Brown lattice) hcp to (complex Brown lattice) phase transformation. Nb-based ordered alloys readily undergo stress induced transformations, making them a common material for shape memory alloys. An application of the method to the description of the coherency 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 DEFORAMED METALS. Robb Thomas (Emeritus) and Lyme Levine, Materials Science and 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 which predict that the dislocation density is a function of the second moment of the dislocation configuration. Results from the critical surface are presented. 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 Beaudoin, SRSM, Gil-sau-Yvette Codex, FRANCE; Florin Petoianu, DAMP; ONERA, Chaireton Codex, FRANCE; Ioane Dacourthial, DAMP, ONERA, Chaireton Codex, 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 interpret fracture of heterogeneous materials in a dynamic phase transition has been made. If models of fronts moving through randomly distributed microstructural features are given satisfactory self-affine regime 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 analyzed with an Atomic Force Microscope on various aluminum 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. Meckel, A. Roos, J Th M De Hesse, Department of Applied Physics, Materials Science Centre and Netherlands Institute for Metals Research, University of Groningen, Groningen, THE NETHERLANDS; H.H. M. Christiansen, 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 diffusivity length the flow stress may decrease rapidly or only slightly in neighboring regions. This will tend to localize the deformation 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 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 Rogovick velocity can attain 2000 K. In the discrete dislocation plasticity approach the crack was described by a distribution of a double spike of dislocations as was put forward by Faddeyev, Nabarro, Bilby and LeBlond in the past. One micron crack in Al was represented by using approx. 500 dislocations and by 114 in Ti. It was concluded that the local heating is experimentally observed in Ti-alloys has to do with fast moving cracks rather than with fast moving dislocations. The former leads to a considerable localized heating 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 Koleckil, Karl H. Zienkiewicz, Christian Stichelberger, 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 all altered with nearly constant material properties. Small strain range, stereophotogrammetric measurements and finite element modeling show that the main influence factors on the scaling effects are concluded: these are the effects of the in-plane and the in-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 (stress, triaxial stress) 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 images taken in the scanning electron microscope. This system provides a three-dimensional model of the deformed fracture surface region consisting of about 10,000 to 20,000 points. The variations of the critical crack tip opening displacement (COD) and the crack tip opening angle (CTOA) have been determined in 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 constraint and the global deformation behavior. It is demonstrated that even for CT specimen under plane strain conditions the global deformation behavior is only depending on the specimen thickness and the stress triaxiality within the process zone are constant. For bend-type specimens under large-scale yielding conditions the stress ratio specimen thickness over length has been found to determine the deformation behavior.

11:15 AM A7.9
VOID NUCLEATION AND VOID DISTRIBUTION EFFECTS ON COALESCENCE IN ELASTIC-PLASTIC SOLIDS. Thomas Pardeon 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. The art approaches used in metal forming modeling and for integrity assessment of cracked or non-cracked structural components typically require (1) the initial porosity, (2) one initial length related to the void spacing, (3) a critical porosity for cracking initiation, (4) a critical porosity for final fracture, 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, it is essential to take
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 simulation. In an extension of Thomson’s ideas, this model directly addresses the mechanism of coalescence by tensile localization 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 are derived after the stress field after the void is 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 COALESCE IN NICKEL. P. David, Parrot II, Univ. of Illinois, Dept. of Theoretical & Applied Mechanics, Urbana, IL; Brian P. Somerset 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 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, disordered 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, void distribution, and interstitial hydrogen. Atomistic data are 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-AC02-94ER54396.*

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

1:30 P.M. A8.1
THE STRUCTURE AND MOBILITY OF DEFECTS FORMED BY ABSORPTION OF CRYSTAL DISLOCATIONS IN INTERFACES IN THE HCP STAUB, J. D. Bacon, R.C. Pond and A. Serra, *Materials Science and Engineering, Department of Engineering, The University of Liverpool, Liverpool, UNITED KINGDOM; *Departament de Matemàtica Aplicada III, Universitat Politècnica 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 c(212) / (103) 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 consequent reconstruction of their cores. In both cases, when a boundary, a broader range of interactions is observed. Included are dislocation transmission from matrix to twin and decomposition in the interface into discrete defects. The simulations demonstrate that the core structures of localized interfacial defects exhibit preferred orientation. In the twin, the ‘basal-prism’ configuration, whereas cores in the tilt boundary resemble [310] twin forms. Dislocation interactions with Burgers vector b, parallel to their host interface can move more effectively in principle, but are mobile only if they have a high thickness h, and their core is wide. Conversely, defects which exhibit high h generally have narrow cores and require complex shears of motion. Applied stress tends to cause core reconstruction of these defects. Defects with high h tend to the interface can move more effectively in some circumstances in response to stress through a climb-compensation mechanism. This can lead to limited mobility of defects in both types of interface, and involves the generation of additional glide interfacial defects due to the stress concentrating effects of the rise of the dislocation core. Activation of the whole system is only possible when the elementary mechanism of motion involves a small number of atoms shifting from one crystal to the other, but is not simply related to h and can occur even when h is relatively large.

2:00 P.M. A8.2
DISLOCATION INTERACTIONS WITH GRAIN BOUNDARIES IN LAMellar TITANIUM ALUMINUM INTERMETALLICS. Jory M.K. Wissig, 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 nanotribic 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-TiAl 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 strengthening of lamellar TiAl alloys. The results of shear transfer across lamellar boundaries between gamma-variant and alpha-variant phase boundaries have been identified and the processes for activation of slip in the lamellar alpha+beta lamellae have been elucidated. Thus the role of defect interactions with lamellar interfaces on the strength and ductility of two-phase TiAl have been assessed. This research is supported by a grant from the National Science Foundation with Dr. Bruce MacDonald as program manager.

2:15 P.M. A8.3

An important step in incorporating grain boundaries into multiscale models 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 NiAl system. Though crystallographically a simple geometry, the interfacial dislocations present in this system, which have Burgers vector of either 1/2[111] or 1/6[112], exhibit a 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. Dept of Energy under contract DE-AC02-94ER54396, in part by the Office of Basic Energy Sciences, Division of Materials Science.

2:30 P.M. A8.4
ATOMIC SIMULATIONS OF DISLOCATION-INTERFACE INTERACTIONS IN THE Cu-Ni MULTILAYER SYSTEM. S. Rosseel and P. M. Huisman*, Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/MML, 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 principal systems, to four kinds of dislocation-interface interactions mediated by the lattice parameter, grain surface and mobile dislocations between adjacent layers. The modulus mismatch introduces a force between a dislocation and its image in the interface. The lattice parameter mismatch generates coreby stress and shear stresses which interact with mobile dislocations. Shear stresses at the interface intersect and cause core reconstruction of dislocations. Defects with large h generally have narrow cores and require complex shears of motion. Applied stress tends to cause core reconstruction of these defects. Defects with h inclined to the interface can move conservatively in some circumstances in response to stress through a climb-compensation mechanism. This can lead to limited mobility of cores in both types of interface, and involves the generation of additional glide interfacial defects due to the stress concentrating effects of the rise of the dislocation core. Activation of the whole system is only possible when the elementary mechanism of motion involves a small number of atoms shifting from one crystal to the other, but is not simply related to h and can occur even when h is relatively large.
3:15 PM A8.5

In recent years the lamellar TiAl with Li structure has been identified as a 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. Atomsim simulations using mobile-body-force potentials were 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 using mobile-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. DMR-96-15298.

3:30 PM A8.6
MECHANISMS FOR SELF-DIFFUSION IN HIGH-ANGLE TILT BOUNDARIES IN FCC METALS. S. Miao, A. Vetter, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM; Y. Mishin, Department of Materials Science and Engineering, Virginia Tech, Blacksburg, VA.

Grain boundary self-diffusion in high-angle tilt grain boundaries in face-centered cubic (FCC) metals has been studied using atomistic computer simulations with semi-empirical potentials. The key problem is to identify the dominant atomic mechanism of diffusion. To this end high-temperature, “kinetic-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, interstitialty 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 MoYBEDEUM: COMPARATIVE ANALYSIS OF EXPERIMENTAL AND THEORITICAL DATA. R. Janiš, T. Ochs, C. Elsasser, Max-Planck-Institut für 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 electronic and structural structures at an STGB [310] [001] caused by tetragonal or hexagonal symmetries and compositions Mo$_x$C$_{1-y}$, are reported. Perspectives for large-scale atomistic simulations (e.g. molecular dynamics) of Carbon segregation to MoYbebedum 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 Mo$_x$C$_{1-y}$ intergranular filaments in tetragonal structures along [25] [310] [001] STGB in MoYbebedum. [1] T. Ochs et al., Phil. Mag. A 1999, in press. [2] J. P. M. Pincus et al., Phil. Mag. A 73, 859 (1996).

4:00 PM A8.8
INFLUENCE OF GRAIN BOUNDARY INTERFACE

3:45 PM A8.9
STRUCTURE ON LIQUID METAL PENETRATION BEHAVIOR. Liping Ren, D.F. Bohr, R.G. Hoggard, 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 under a liquid metal. In severe cases, the LME failure can occur even under no applied stress condition and is usually time-dependent, e.g. Ga embrittlement in Al, 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 to study the effect of grain boundaries interfaces. In the experiments, Ga penetration rates were measured by in-situ TEM and SEM observation. Preliminary results indicate that the structure of grain boundaries and interfaces, especially those containing defects, significantly affect Ga penetration rates. Ga was deposited at liquid Ga at a constant temperature of 540°C and the penetration rates were measured by in-situ TEM and SEM observation. The support of the US Department of Energy through grant DE-FG08-87ER45287 is gratefully acknowledged.

4:15 PM A8.10
ATOMIC 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, we establish that a grain size of about 10 nm in diameter produces the same minimum grain size as a single crystal. Next, we observe the effect of varying the temperature on grain boundary migration rates. The observed migration rates are consistent with the experimentally observed rates observed in TEM measurements. The support of the US Department of Energy through grants DE-FG08-87ER45287 is gratefully acknowledged.

3:45 PM A8.11
DIRECTIONAL GRAIN BOUNDARY TRIPLE JUNCTION EMBRITTLEMENT: AN ATOMIC SIMULATION STUDY. M. Umezawa, S. S. Sirovich, E. S. Shvidlerman, and Guenter Gottstein, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI; *Princeton Materik Institute Instituute, Princeton University, Princeton, NJ; **Institute of Solid State Physics, Russian Academy of Sciences, Moscow, Russia; †Institut für 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 microstructures. The dynamic triple junction angle is measured as the half-loop migration reaction of the grain boundary triple junction mobility. Additional simulations are performed using a geometry where identical triple junctions move in the opposite directions (invoking the destruction of the symmetrical tilt boundary, which now forms the front of the LME failure), finding 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 the junctions which 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 mobility with temperature is also presented. For high temperatures, the triple junction migration is found to be an activated process.
TWINNING DEFORMATION IN MARTENSITE MICRO-STRUCTURE. Udorn Nia, G. and Praveen, A. K., 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-bcc transition. The microstructure is composed of (101) twin boundaries and boundary dislocations which sometimes spread across the twins forming stacking faults. A series of such equilibrium microstructures subjected to discrete, increasing £ 1121 £ 101 shear strain. The stress-strain curve has stick-slip behaviour with yield stress of £ 5.5GPa and yield strain of £ 3.8%. Deformation occurs through twinning dislocations; straight perfect twin boundaries do not move.

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

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

We have studied impurity atoms in the high-angle (100) twist grain boundaries 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 2000 atoms. The study is motivated by recent progress in nano crystalline diamond growth. Structural relaxation calculations were carried out for several grain boundaries and final relaxed configurations of the impurity atom in the grain boundary. Various impurities 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 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 ALU(MNI) GRAIN BOUNDARY. Gang Lu, Nicholas Kousisis, 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 6 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 were 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 behaviour and the corresponding electronic structure with 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. Parascak, R. Miller, R. Phillips, Division of Engineering, Brown University, Providence, RI; Department of Mechanical Engineering, University of Saskatchewan, Saskatoon, CANADA

We investigate the atomistic-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-symmetry boundaries and 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 MIcroSCOPICALLY INDUCED Failure EVOLUTION AND GLOBAL FAILURE IN POROUS CRYSTALLINE AGGREGATES. W. M. Azzam, 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 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, 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 that granular 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. Yari Moshii, 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 quasiharmonic approximation. From 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 offset-stochiometry on grain boundary properties, such as cohesive strength and diffusion, is analyzed.

A9.6 MONTE CARLO INVESTIGATIONS OF Σ5 TILT GRAIN BOUNDARY IN ALUMINUM. Peter Ballo, Slovak Technical University, Dept. of Physics, Bratislava, SLOVAK REPUBLIC; Nicholas Kousisis, Gang Lu, California State University Northridge, Dept. of Physics, Northridge, CA

The microscopic mechanism for the sliding of the Σ 5 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 results, as well as with the available 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 happen during the entire GB sliding process. It is evident that in aluminum the GB migration depends sensitively on the combined action of the GB sliding (and migration) which 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
A0.10 SURFACE RELAXATIONS OF ALUMINUM SIMULATED BY BOND ORDER POTENTIALS. Shigeto Nishihara, Sadakichi Ogushi, Hiroshi Adachi, Kyoto Univ., Dept. of Materials Science and Engineering, Kyoto, JAPAN; Osaka Univ., Dept. of Electrical and Electronic Engineering, Gifu, JAPAN.

For the real-time simulations of the defect structures at atomic level, reliable interatomic potentials are indispensable. However, the oscillatory damped behavior observed on the perfect surface defects have been hardly reproduced by the simple empirical potentials. Very recently, we have performed the simulations on a multilayer surface relaxations of aluminum by bond order potentials with the surface 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 method 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.

A0.11 STRUCTURE AND BONDING OF THE RHOBOHEDRAL TWIN INTERFACE IN \( \alpha \)-Al\(_2\)O\(_3\). A. G. Merinopoulos, C. E. Watson, Max-Planck-Institut fuer Metallkunde, Stuttgart, GERMANY.

We have studied the local atomic structure and chemical bonding of the rhombohedral twin interface in \( \alpha \)-Al\(_2\)O\(_3\) 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 HREM observations. These experimental observations, however, could not make decisive conclusions about the interfacial structure because only images of two-dimensional projections along the [2\(\bar{1}\)0] axis were analyzed. For the symmetrical (01\(\bar{1}\)2) and (01\(\bar{1}\)2) twin orientation, the corresponding dichromatic images lead to a number of possible 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 predictions of the empirical shell-model calculations and complementing the HREM observations. Furthermore, detailed insights into the local electronic structure at the interface are accessible. [1] T. Geipel et al., Acta mater. 42, 1367 (1994). [2] F. R. Chen et al., Phil. Mag. A 72, 529 (1995).

A0.12 IDENTIFICATION OF 3D BOUNDARIES FROM 3D ATOM PROBE DATA, AND CORRELATION OF ATOMIC DISTRIBUTIONS WITH POSITIONS OF INTERFACES. Olof C. Hellman, Jan Van den Broek, Dieter Ideus, Ing Räisänen, 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 calculated 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 resolution of the analysis.

A0.13 CRACK BEHAVIOUR AT BI-MATERIAL INTERFACE - A MIXED ATMOSPHERIC/CONTINUUM APPROACH. Arun R. Pillai, Ron M. Miller, University of Saskatchewan, Department of Mechanical Engineering, Saskatoon, CANADA.

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Interfacial defects like grain boundaries and phase boundaries play an important role in the mechanical behavior 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 in a micro-scale with the goal of elucidating the interaction between the microscopic elastic fields and the macroscopic crack tip phenomenon. We study a bimaterial interface crack at the atomic level using the Quasicontinuum (QC) method. The QC method incorporates the effective atomic force 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)611-642]. The QC method treat critical regional like the crack tip atomically and regions away from the tip as a continuum thereby reducing the degrees of freedom and simplifying the application of boundary conditions. The underlying atomic model used is the Embedded Atom Method [J. S. Dues and M. J. Baskes, Phy Rev B, 29,p443]. 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 behavior of the bimaterial crack. This behavior 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.

A0.14 EMBEDDED ATOM METHOD AND FINITE ELEMENT ANALYSIS OF ALUMINUM-SILICON INTERFACE FRACTURE. K.A. Gall, M.F. Horstemeyer, Sandia National Laboratories Livermore, CA; M. Baskes, Los Alamos National Laboratories Los Alamos, NM.

Fracture of silicon particles and interface peeling of the Al-Si interface has been observed during the mechanical loading of an AlS56 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 [100][100]Al interface is considered. In an unloaded and reduced state, the EAM predicts that the interface between the Al and the Si is ineinherent 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 scale 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 time increment due to excessive plasticity in the Al at the micro-scale whereby defects 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-AC04-94AL8500.

A0.15 SELF-AFFINE MEASUREMENTS ON FRACTURE SURFACES OF PLASTIC MATERIALS BY AFM. Edgar Reyes, Carlos Guerrero, Virgilio González and Mónica Hinostroza, Doctorado en Ingeniería de Materiales, Facultad de Ingeniería Mecánica y Eléctrica, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, Nuevo León, MÉXICO.

In this work, self-affinity of fracture surfaces of a semi-crystalline and at amorphous polymers were studied over a range of scales using a contact mode atomic force microscope (AFM). Before the measurements, the optimal operating conditions on the C-AFM were fixed. These conditions allowed us to obtain height profiles on several zones of the fractured sample. Using these measurements, the mean Hurst exponent [1], was estimated through the variable bandwidth method. A value of $H=0.988$ was obtained for $i$-PP over two decades of length scales and $H=0.865$ for PS over one decade. These results are in agreement with the values reported in the literature for other materials, mainly metals and ceramics. In addition, it is proved that, choosing the adequate operating conditions, reliable roughness measurements can be done on fracture surfaces of plastics materials using the C-AFM.

A0.16 ATOMIC SCALE SIMULATIONS OF CRACK INITIATION IN SILICON. Antti Maki-Jaske, Kimmo Kraki, Antti Koronen 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 by the usual method of many-body potential energy model, 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 behavior 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 angles and distances of 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 small, 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.

A0.17 A PARTITIONED-PROBLEM APPROACH TO MICRO-STRUCTURAL MODELLING OF A GLASS-CERAMIC. Anthony C. Finches-Cripps, CSIRO Division of Telecommunications and Industrial Physics, Sydney, AUSTRALIA.

The indentation response of a micro-containing glass-ceramic is studied. In this type of material, the indentation cracks which normally occur in brittle materials loaded with a hard spherical indenter is suppressed in favour of distributed surface damage indicating plastic yield. Theoretical analysis, finite-element modeling and experimental results are used to establish a connection between the microstructural behaviour of the material and damage events occurring on the microstructural scale. This is achieved by first determining the microscopic material properties, such as yield stress and strain-hardening index, in terms of the microstructure. These properties are then used to predict the 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.

A0.18 IDENTIFICATION OF MULTIPLE, SIZE DEPENDENT, PHASE TRANSFORMATIONS DURING POINT LOADING OF SILICON. A. B. Miao, T. P. Weihs, D. van Heerden, The Johns Hopkins University, Department of Materials Science & Engineering, Baltimore, MD, J. B. Miller, Oxford University, Department of Materials, Oxford, UNITED KINGDOM.

During point-loading (indentation) of silicon we used a unique combination of in situ electrical and acoustic measurements and ex situ transmission electron microscopy to identify the size-dependent 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, BCC, phase while for larger volumes it is amorphous silicon. The size dependence is explained by considering two stress fields, one with contact size and how interfacial effects between the silicon substrate and the BCC phase determines 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 rhombohedral, RB phase) is observed. The multiple phase transformations observed experimentally are compared to quasi-continuum models of nanoincipient in silicon and the measured electrical properties are used to verify first-principles calculations for silicon's high pressure phases.

A0.19 RESIDUAL STRESSES AND CRACKING IN ALUMINA. V.W. Vedala, S. J. Hill, Sandia National Laboratories, Albuquerque, NM.

Residual stresses arise in ceramics during processing as a result of thermal expansion mismatch and crystallographic anisotropy across the grain boundaries. The magnitude of these stresses can be
very high (206-300 MPa) and may cause spontaneous microcracking during the processing of these materials. The microstructural level stresses are likely to play a significant role in crack initiation and propagation under macroscopic loading too. The magnitude of residual stresses in alumina was predicted using object-oriented finite element analysis and experimentally determined orientation 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 microcracks and predicted stresses at the grain boundaries that were formed in simulations were compared with 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-AC04-94AL85000.

A0.20 DISPERSE MEASUREMENTS OF VELOCITY IN HETEROGENEOUS MATERIALS, M.D. Keaden, W.M. Trott, J.R. Argy, M.R. Bier, N. Castellanos, L.C. Ghilani, Sandia National Laboratories, Albuquerque, NM. An optically-seeing 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 for the measurement of the mesoscale dynamic response of shocked materials has been demonstrated on several different classes of heterogeneous materials, including: foam, glass-reinforced polymer, and pressed, granulate-sand (high-explosive composite). This presentation will be focused on the results of plan-impact, shock wave experiments performed on pressed, granulate-sand 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 mesoscale dynamic processes, and (iii) critical evaluations of 3-D numerical simulations for the particular experimental configuration that incorporates physics-based models to treat the grain-boundary properties and grain-boundary interactions. The developments described 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.

A0.21 HIERARCHICAL LENGTH-SCALE INFLUENCE ON CRACK PROPAGATION IN MICROCOMPOSITES. Luke N. Brewer and Vasanak P. Drawzi, Northwestern University, Dept. of MSE, Evanston, IL. Fracture of materials presents a classic microstructure-property correlation problem where crack propagation is affected by virtually all microstructural length-scales from the finest bonding 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 researched, experimentally solidified [1], the effect of oxide-oxide and oxide-metal materials (e.g. NiO-ZrO2, CoO-ZrO2, W-ZrO2, etc.) as model macrocomposite 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). Manipulation of crack paths, especially those under macroscopic stress fields 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 its properties and 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 DSC microcomposite systems. It will be argued that the experimental and theoretical electron microscopy have advanced further enough to provide significant clues to both the lengthscale 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 FRAC.TAL CHARACTERIZATION OF TNI FRACTURE SURFACE. L. V. Johnson, Benet Laboratories, US Army TACOM-ARDEC, Waterlief, NY, Y. D. Lapengo, 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 reproduced by computer using an electron micrograph 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 0.816 μm to 0.0 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 structure 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 scaling can be unambiguously derived from the TNT fracture surface. This provides important information that is not evident in the analysis of individual surface sets.

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/m2. 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. Kalin, Aichiro Nakano, Priya Vashishtha, 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, Yamanashi 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 Al2O3. Dependence of crack propagation on the existence of the oxide-metal interface, and the continued oxidation of fracture surfaces is presented. The effects of charge transfer, structural correlations, and stress near the crack are analyzed. Work supported by AFOSR, DOE, LENS, NASA, NSF, and USCL SUMURI from DARPA.


A9.26 MICROSTRUCTURAL FAILURE MODES IN NANO-GRANITE THIN FILMS: NUMERICAL MODELS AND EXPERIMENTS. J. N. Braccon, A.J. Griggs, M.A. Zikry, J. Kindsvater, North Carolina State University, Department of Mechanical and Aerospace Engineering, Raleigh, NC. A multiphase 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 nanosized 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 evolved 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, geometric 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.