SYMPOSIUM W
The Limits of Strength in Theory and Practice
November 28 – 30, 2000

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*Invited paper
SESSION W1:
Chair: J. W. Morris, Jr.
Tuesday Morning, November 28, 1990
Fairfax B (Sheraton)

8:30 AM W1.1
LATTICE INSTABILITY AND LIMITS OF STRENGTH IN THEORY AND ATOMIC SIMULATIONS
Ja Li, Sidney Yip, Massachusetts Institute of Technology, Dept. of Nuclear Engineering, Cambridge, MA.

We examine the theoretical basis and simulation techniques for understanding the response of crystalline lattice to critical stress loadings at finite temperatures. Various derivations now exist giving the stability criteria for homogeneous material in terms of load-dependent elastic stiffness coefficients. These criteria provide upper bounds on the material's strength, approachable sometimes in indentation hardness experiments. The extension of homogeneous deformation to finite wavelength is the analysis of phonon soft mode for a strained stressed elastic system in the neighborhood of the soft mode. We will present lattice dynamical results obtained using model potentials for a variety of solids [Mg, Cu, Mo, Si, SiC, SiO$_2$, and ZrC] under hydrostatic, shear, and uniaxial loadings. We find that simple lattices often fail by elastic instabilities (k=0 modes), whereas the binary lattices mostly fail by soft modes at Brillouin zone boundaries. The latter is often interpreted as the breaking of heteropolymer bonds driven by the local competition for chemical affinity. To study the lower limits of strength, one must deal with defect mobility. However, an acute problem for atomic simulations is the lack of a sound measure of how the defect is driven, since during the available time the size of atomic scale plasticity, not to mention the concept of stress field itself, may not be applicable. We propose a local measure of the thermodynamic driving force for the evolution of an isolated defect which focuses on energy considerations in much the same spirit as the integral in fracture mechanics. This concept is applied to the study of strength and deformation of Cu in various idealized microstructures by molecular dynamics simulation.

9:00 AM W1.2
ATOMISTIC SIMULATIONS OF CRACK PROPAGATION IN SiO$_2$ UNDER EXTREME CONDITIONS OF PRESSURE AND TEMPERATURE. M.J. Caturela, A. Kubota, T. Lenosky, V. Bulatov, T. Dux de la Rubia, M. Feit, Lawrence Livermore National Laboratory, Livermore, CA.

The mechanical strength of silicon glass is of great importance for industrial and scientific applications, including semiconductor processing and laser optics damage issues. In particular, silicon optics used to focus UV laser light can undergo damage that grows with subsequent laser pulses. Mitigation of the damage growth is of extreme importance for the National Ignition Facility under development at Lawrence Livermore National Laboratory. For this application it is important to understand the time-resolved atomic-scale mechanism of crack growth in silicon under extreme conditions of pressure and temperature. For this purpose we have modified our parallel molecular dynamics code MDCASK by including fast multipole expansion algorithms to describe long-range Coulombic interactions. We compare several empirical interatomic potentials with ab initio (GGA) calculations under different loading tests in order to select an empirical potential that is most suitable for this study. We show interesting trends in SiO$_2$ fracture properties of pre-existing cracks as a function of varied conditions, including large temperature and pressure gradients induced by high localized absorption of UV laser light. This work was carried out under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract W-7405-Eng-48.

9:15 AM W1.3
DIRECTIONAL ANISOTROPY IN THE CLEAVAGE FRACTURE OF SILICON. Rubén Pérez and Peter Gumbsch, Universidad Autonoma de Madrid. Departamento de Fisica Teorica de la Materia Condensada, Madrid, SPAIN, Max Planck Institut für Metallforschung, Stuttgart, GERMANY.

Total-energy pseudopotential calculations are used to study the cleavage fracture anisotropy in silicon. This full quantum mechanical analysis provides an accurate description of the nonlinear forces acting on the crack tip atoms. A fixed boundary approach is used to enforce the boundary conditions representing the crack field. The influence of the fixed boundary is determined through the scaling of the results with system size and with the changes with the relative position of the crack elastic field singularity and the atomic position of the crack tip. The simulations show that the bond breaking at the crack tip proceeds differently for the different crack orientation. Crack tip bonds smoothly lengthen with increasing load and cracks propagate easily on [111] and [110] planes provided crack propagation proceeds in the (110) direction. This continues breaking process mimics what one would expect from continuum theory and therefore results only in a small lattice trapping. In contrast, if the crack is driven in a [001] plane the continuum breaking process is discontinuous: the crack tip bond length remains almost unchanged until the external load reaches a critical value at which the bond abruptly breaks. This bond breaking is associated with pronounced relaxations of a small number of atoms surrounding the crack tip. The origin of the discontinuous behavior can be traced back to some bond sharing between the crack tip bond and the neighboring bond, which effects shields the crack tip bond from the applied load and results in a larger load required. The different lattice trapping for different crack propagation directions can explain the experimentally observed cleavage anisotropy in silicon single crystals.

9:30 AM W1.4
INFLUENCE OF CRYSTALLINE SYMMETRY ON ELASTIC STABILITY AND BIFURCATION PHENOMENA AT FINITE STRAIN. Frederick Mittleman, Univ of California, Santa Barbara, CA.

The theoretical response of metals to various modes of loading at finite strain is examined. Particular attention is given to the topic of elastic instabilities at points of bifurcation, as well as to post bifurcation phenomena leading to phase change or material failure, as predicted by elastic stability theory. The mechanical response including theoretical strengths, is strongly influenced by crystalline symmetries and associated bifurcation behavior. Prominently featured are computational results based on an embedded atom method that is formulated to reproduce, identically, empirical values of the three second order elastic moduli (c_{11}, c_{12}, and c_{44}) and the six third order elastic moduli (c_{111}, c_{112}, c_{123}, c_{144}, c_{166}, and c_{566}) of 12 cubic metals [Al, Cu, Mo, Na, Li, K, Rh, Nb, Fe, Ni, Au, and Ag]. This formulation ensures that the both the linear (harmonic) and non-linear (anharmonic) response of the metals is represented in the computations. Examples of both lattice static and molecular-dynamic results are presented.

10:00 AM W1.5
COMPUTATION OF THE IDEAL STRENGTH. David Roundy, Marvin L. Cohen, Dept. of Physics, Univ. of California Berkeley, Lawrence Berkeley National Laboratory, CA.

The ideal strength is the upper limit of the strength of a material. Advances in computing have made possible increasingly accurate calculations of the ideal strength, but there are challenges in imposing a desired stress tensor. We will discuss the methods used in calculations of the ideal and discuss the results of recent ab initio calculations of the ideal tensile strength as well as the ideal shear strength of various materials.

11:00 AM W1.6
CORRELATION OF TOPOLOGY OF CHARGE DENSITY WITH ENERGETICS IN SHEAR AND CLEAVAGE DEFORMATIONS IN FCO METALS. Nicholas Kuzmany, M. H. Rieder, and E. Colla, California State Univ. Northridge, Dept of Physics, Northridge, CA, Mark Eberhart, Chemistry and Geoscience, Colorado School of Mines, Golden, CO.

We have employed ab initio total-energy electronic structure calculations, based on the full potential linear muffin tin orbital method, to evaluate the energetics and topology of the charge density in shear and cleavage deformations in Al, Ag, and Ir, exhibiting different mechanical properties. We will present a correlation between phase fault and cleavage energetics with the shape of the charge density in the neighborhood of its critical points, i.e., the anisotropy of the principal curvatures of the charge density parallel and perpendicular to the bond path. This anisotropy factor is directly related to the bond stiffness and the bond stiffness gradient for both breaking and forming bonds. We show that one or both principal curvatures perpendicular to the bond path vanish at the unstable stacking fault configuration. Supported by U.S. Army Research Office.

11:15 AM W1.7
THEORETICAL TENSIILE STRENGTH IN METALS AND INTERMETALLICS. M. She, L. G. Wang, M. Frink, Institute of Physics of Materials, Academia Sciences of the Czech Republic, Brno, CZECH REPUBLIC, V. Vittek, Department of MSE, University of Pennsylvania, Philadelphia, PA.

Fully self-consistent ab initio electronic structure calculations of the theoretical tensile strength in metals and intermetallics loaded uniaxially along several crystallographic directions are performed using the full-potential LAPW method. It turns out that the theoretical tensile strength and lattice misfit of higher intermetallics are closely connected with the presence or absence of higher-symmetry structures along corresponding deformation paths. Total energy
calculations show that all higher-energy cubic structures studied are locally unstable with respect to tetragonal and/or trigonal deformation modes. In intermetallics, there may or may not be symmetry-directed energy extremas corresponding to cubic lattices depending on the atomic ordering. However, other energy extremas along the deformation paths besides those required by symmetry occur. Configurations corresponding to energy minima on the deformation paths may represent metastable structures that can play an important role in interfaces and other extended defects. As specific examples, tensile strengths of single-crystalline tungsten, NaI and MgSO₄ loaded uniaxially along principal crystallographic directions will be discussed.

11:45 AM W1.8
STRAIN-RATE-DEPENDENT COOPERATIVE DISLOCATION GENERATION IN CRYSTALS AT FINITE TEMPERATURES: APPLICATIONS TO THE YIELDING OF WHISKERS AND THE DRITTE-DUCTILE TRANSITION. M. Klement, V. Vitek, R. Folk and D.P. Pope, Department of MSE, University of Pennsylvania, Philadelphia, PA.

A new strain-rate dependent mechanism of dislocation generation that can become active suddenly above a critical temperature is described. This mechanism is a thermally driven, stress assisted cooperative instability of many dislocation loops that leads to an outburst of dislocation activity above the strain-rate dependent critical temperature. In contrast to the large temperature-independent energy barrier associated with the thermal activation of individual dislocation loops, this process is marked by an activation barrier that decreases dramatically with temperature becoming zero at the critical temperature. The strain-rate dependence originates from the glide of pre-existing and thermally nucleated dislocations below the critical temperature. We demonstrate by theory and experiments that the onset of yielding in a crack-free crystal with a very low dislocation content (Si in our study) is remarkably similar to the brittle-to-ductile transition in a pre-cracked crystal of the same material.

This research was supported by U.S. Air Force Office of Scientific Research grant F49620-86-1-0245.

SESSION W2
Chair: Peter Gumbsch
Tuesday Afternoon, November 28, 2000
Fairfax B (Sheraton)

130 P.M. #W2.1
PREDICTABILITY OF INTRINSIC STRENGTH. T. Suzuki* and H.O.K. Kirchner**, *Institute of Industrial Science, University of Tokyo, Tokyo, JAPAN. **Institut de Sciences des Matériaux, Université Paris-Sud, Orsay, FRANCE.

So far dislocation theory has served in the interpretation of macroscopic and microscopic observations in crystal plasticity, the aim being an understanding of the evolution of the microstructure. For a long time the approach has remained descriptive rather than predictive. Only recently a wealth of microscopic plasticity data on bcc metals [1] and semiconductors [2,3] have been consolidated into a universal relation describing the dependence of the critical stress on dislocation content. This is possible as far as the deformation mechanism is an intrinsic lattice one (the Peierls process). With such universal scaling laws one can predict the strength of a crystal for which the lattice and elastic constants are known, but for which, for various reasons, plasticity data are not available, for example platinum (ε-Pt) or boron-nitride (c-BN).


2:00 PM W2.2
LOWER LIMITS OF STRENGTH IN BCC METALS AT LOW TEMPERATURES. R. Gibala, University of Michigan, Ann Arbor, MI.

The flow stress of high purity body centered cubic metals at low homologous temperatures, e.g. below about 0.15 of the absolute melting temperature, or equivalently high strain rates is governed by the relatively low intrinsic mobility of screw dislocations in the bcc crystal structure. By contrast, the mobility of edge dislocations is much higher and affords plastic deformation at correspondingly lower flow stresses. The large difference in critical flow stress for edge and screw dislocations can be demonstrated in many ways. In this paper, we examine several such methods, especially experiments in which surface films may be used to afford preferential nucleation of dislocations at the film-substrate interface and generation into the bcc substrate under applied stress. Experiments on high purity Group V and VI metals and selected solid solution alloys are described.

2:15 PM W2.3
STATIC AND DYNAMIC ELASTIC INTERACTION BETWEEN DISLOCATIONS AND POINT DEFECT CLUSTERS IN FCC METALS. Lizhi Sun, University of Iowa, Dept of Civil and Environmental Engineering, Iowa City, IA. Jimming Huang, Near M. Gloniemi, University of California at Los Angeles, Dept of Mechanical and Aerospace Engineering, Los Angeles, CA.

Under extreme environmental loading conditions, such as those achieved in metals irradiated by neutrons, electrons, particles or laser light, and in metals quenched from high temperatures or subjected to high-shear deformation by shock loading or high strain rates, copious concentrations of point defects and defect clusters are produced. The interaction of dislocations with point defects and their clusters results in significant modification of the materials strength. In this work, we analyze the interaction energy and configurational forces arising between dislocations and such defect clusters. A new analytical solution to the interaction energy between glide dislocations and vacancy clusters in the form of perfect Stacking Fault Tetrahedra (SFT’s) in FCC metals is first presented. This is complemented by numerical solutions for the interaction energy of truncated static SFT’s. Displaced Dislocation Dynamics (DD) simulations are then used to determine the necessary critical flow stress, accounting for dislocation deformation during its interaction with SFT’s. The mechanisms of dislocation interaction with interstitial defect clusters are also analyzed by DD. It is demonstrated that substantial dislocation deformation occurs during such close-range interactions, and that the critical flow stress is achieved when dislocations reach a symmetry-breaking configuration, allowing for line tension effects to aid in dislocation breakaway from interstitial defect clusters.

2:30 PM W2.4
PEIERLS STRESS AND LATTICE RESISTANCE IN FCC METALS. David L. Olmsted, Kedar Y. Hardiker, Rob Phillips, Division of Engineering, Brown University, Providence, RI.

There are only a few results available of atomistic computations of Peierls stress for fcc metals. By comparison, there are many more atomistic computations for bcc metals, as well as mixed discrete-continuum computations of the Peierls-Nabarro type for fcc metals. One of the reasons for this is the low Peierls stresses in fcc metals. Because atomistic computations of the Peierls stress take place in finite simulation cells, image forces caused by boundaries must either be relaxed or corrected for if valid results are to be obtained. We present computations of the line energies, Peierls stress and lattice resistance curves for screw, edge and mixed character dislocations in aluminum, based on an embedded atom potential. As far as we are aware, these are the first atomistic computations of the Peierls stress of edge or mixed dislocations for an fcc metal.

2:45 PM W2.5

Using a new, first principles based, Embedded-Atom-Model (EAM) potential for tantalum (Ta), we have carried out atomistic simulations to investigate the core structure, core energy and Peierls energy barrier and stress for infinite and straight 1/2<111> screw dislocation. Equilibrium core structures were obtained by relaxation of dislocation quadrupoles with periodic boundaries. We found that the equilibrium dislocation core has three-fold symmetry and spreads out in three <112> directions and <110> planes. Core energy per Burgers vector b was determined to be 1.36 eV/ b. We studied dislocation motion and annihilation via Molecular Dynamics simulations of a periodic dislocation dipole cell, with <112> or <110> dipole orientation. In both cases the dislocations move in zigzagging on primary <110> planes. Atoms forming the dislocation cores are distinguished based on their atomic energy. In this way we can accurately define the core energy and its position not only for equilibrium configurations but also during dislocation movement. Peierls energy barrier was computed to be ~0.08 eV/b with a Peierls stress of ~0.03 u, where u is the bulk shear modulus of perfect crystal. The preferred slipping planes at low temperature are <112> directions and <110> planes. Dislocation core defects, flip and kink, have been constructed and energetically relaxed. Preliminary computation results showed that formation energy of a flip is ~0.57 eV and formation energy of kink is ~0.62 eV. It is also found that flip
is a rather stable defect while kink can move freely along dislocation line. We attributed the lower experimental flow stress of dislocation to the high mobility of kink.

3:30 P M W2.6
DEPRESSING FRACTURE FRACTURE OF IRON BY ULTRA GRAIN REFINING. Kotsuki Naga, National Research Institute for Metals, Honsi, JAPAN.

Low temperature brittleness is thought as an inevitable phenomenon for low-carbon steels when some alloying elements like Ni are added. However, an empirical equation predicts very low ductile-to-brittle transition-temperatures (DBTT) for low carbon ferrite-perlite steels that should have ultrafine grain sizes smaller than 1 micron. Industrial steels with the grain sizes of 10 micron order show the DBTT higher than 200 K. The author's group has successfully fabricated thick specimens containing the ultrafine grains large enough to take full-size impact test pieces for a low carbon steel. The DBTT of such steel is 0 K. For this steel we think that the yield stress is very low comparable to that for the 9% Ni steel. The strength of the steel was almost doubled compared with that of the starting material with a 20 micron ferrite and perlite structure.

4:00 P M W2.7
THE LIMIT OF STRENGTH AND DUCTILITY. Zhen Guo and J. W. Morris, Jr., Berkeley, CA.

Computations of the limits of strength in tension suggest that for metals necessarily cease on [100] at a tensile stress of about 0.88E(-100) while for metals cease if at all on [110] at a tensile stress of 0.7E(-100). Further deformation analyses of the normal stress in the stress concentration region ahead of a crack suggest that the peak tensile stress may reach four times the yield strength or more, depending on work hardening behavior. Taking these results together, we can estimate the highest values the yield strengths of typical metals and alloys could reach without forcing brittle fracture. We shall report results for a number of materials, concentrating on steel and aluminum. Interestingly, preliminary calculations suggest that the "ductile fracture limits" is exceeded by a number of existing alloy steels, but is not approached in structural aluminum alloys.

4:15 P M W2.8

Grain refinement is a promising way to enhance both the strength and the toughness of structural steels. Recently, it is known that ultrafine ferrite of around 1µm can be obtained by heavy deformation at just above Ar3 temperature during cooling of austenite. But the mechanism of ultrafine grain refinement is not clear till now because the amount of deformation is far beyond the usual one. In this paper, flow curve during deformation, dilatation, and microstructure were investigated in order to understand the mechanism of the grain refinement. And it was found out there is a strain induced dynamic transform during deformation of supercooled austenite to ultrafine ferrite by the nucleation of ultrafine ferrite during heating just after deformation. The grain growth rate of ferrite transformed during deformation was slower than that of ferrite transformed during cooling after deformation. And the effect of deformation temperature on amount of deformation and material grain size on the grain refinement and the mechanical properties was investigated in a single heavy reduction and repeated light reductions.

4:30 P M W2.9
LOW-TEMPERATURE, LARGE STRAIN DEFORMATION BEHAVIOR OF NANO-CRYSTALLINE PALLADIUM BY MOLECULAR-DYNAMICS SIMULATION. Y.I. Yoon, B.D. Wolf, S.R. Plimpton, Argonne National Laboratory, Argonne, IL., Gleiter, Forschungszentrum Karlsruhe, Karlsruhe, GERMANY.

Molecular-dynamics simulations are used to elucidate the low-temperature, large deformation behavior of nanocrystalline film Pd up to about 90% strain with no sign of crack nucleation. The simulated model system contains 16 randomly oriented grains of uniform size and shape arranged in a periodically repeated, infinite cubic box. The response of the system to a constant, uniaxial applied stress at a temperature of about 20% of the melting point reveals two stages in the deformation process. First, up to about 10% strain the system deforms uniformly, with a constant strain rate and a grain-boundary-deformation mechanism. On further straining, the accumulated stress in the system gradually relaxes as evidenced by a rapidly increasing strain rate, until a total strain of about 70% is reached at which the strain rate decreases again. A dislocation deformation mechanism is associated with the nucleation of new grains from the triple junctions; the underlying mechanism involves stress-induced amorphization of the triple junctions followed by recrystallization and the formation of new grains. As evidenced by the reduction in the strain rate, the newly formed grain microstructure, containing more spherically shaped but smaller grains, apparently accommodates the highly elongated system shape better than the original microstructure with the highly elongated grains. This mechanism of grain refinement during plastic flow might provide an explanation for the appearance of spherical grains even after rather substantial plastic elongation under uniaxial stress.

# Work supported by the U.S. Department of Energy, Office of Science, under Contract W-31-109-Eng-38.

4:45 P M W2.10
PHASE FIELD MICROELASTICITY APPROACH TO DYNAMICS OF DISLOCATIONS SYSTEM. Yu. U. Wang, Rutgers Univ, Dept of Mechanical and Aerospace Engineering, Piscataway, NJ; Yongmei Jin, Rutgers Univ, Dept of Ceramics and Materials Engineering, Piscataway, NJ; Alberto Volpi, Rutgers Univ, Dept of Mechanical and Aerospace Engineering, Piscataway, NJ; Armen G. Khachaturyan, Rutgers Univ, Dept of Ceramics and Materials Engineering, Piscataway, NJ.

The elastic strain and the strain energy generated by the dislocation system of arbitrary geometry are formulated in terms of the Phase Field Microelasticity (PFM) theory previously proposed by one of the authors. The exact solution for the strain energy is presented as a functional of the phase fields describing any spatial configuration of dislocations. Incorporating the PFM solution in 3-D Phase Field kinetic model results in the kinetic equations governing an evolution of an arbitrary dislocation pattern under applied stress. The proposed model automatically takes into account the "short-range interactions", such as multiplication and annihilation of dislocations as well as a formation of various metastable microstructures involving dislocations and defects. This model, as a consequence of the PFM, does not impose prior constraints on dislocation patterns formed during the evolution. The Phase Field Dislocation model is used to simulate the mechanical behavior of dislocations during plastic flow. Nucleation and critical flow stresses for dislocations are studied. Examples of simulation of the 3-D for system are discussed.

SESSION W3
Chair: Naor M. Gloniem
Wednesday Morning, November 29, 2000
Fairfield B (Sorrento)

8:30 AM W3.1
TECHNICAL AND REGULATORY DEVELOPMENTS NEEDED TO ENABLE APPLICATION OF MASTER CURVE TECHNOLOGY TO THE FRACTURE INTEGRITY ASSESSMENT OF COMMERCIAL NUCLEAR POWER REACTORS. Mark Kirk, U.S. Nuclear Regulatory Commission, Rockville, MD.

The Master Curve, as introduced by Wallin and co-workers in 1984, has evolved into a mature technology for characterizing the fracture toughness transition of ferritic steels. Considerable empirical evidence provides testament to the robustness of the Master Curve approach. However, in 1997, the NRC staff detailed several technical issues requiring resolution prior to staff acceptance of applications of Master Curve technology to the fracture integrity assessment of nuclear RPVs. Current and recently completed research programs sponsored by both the NRC and EPRI focus on closure of these issues. This paper reviews the issues detailed in 1997, comments on their continued relevance in light of recent research results, and details areas where either additional research or a change/research focus is warranted.

9:00 AM W3.2
DISCRETE DISLOCATION SIMULATION OF THIN FILM PLASTICITY INCLUDING THE EFFECT OF DISLOCATION SOURCES. Berghard von Blanckenhagen, Peter Gumbsch, Eduard Arzt, Max-Planck-Institut für Metallforschung, Stuttgart, GERMANY.

The flow stress of thin metal films is much higher than the flow stress of the corresponding bulk material and scales approximately with the inverse film thickness. This was shown in many experiments but the mechanisms are not yet fully understood. A dislocation dynamics simulation is used here to investigate dislocation motion in thin metal films. A thin polycrystalline film with columnar grains on a substrate was simulated. As a first step, grain boundaries are introduced as impenetrable obstacles for the dislocations. In analogy to the Hall-Petch model it is assumed that flow in a neighbouring grain is achieved if the force on the grain boundary exceeds a certain critical value. Dislocation sources are included explicitly. Work hardening is contained in the back stress of the dislocations on the
source. The calculations show that the film thickness and grain size have to be treated equivalently, the smaller of the two controlling the flow stress. It was found that the optimum orientation in the film thickness is approximately one fourth of the film thickness (or grain size) if the source is of Frank-Read type and if a source is required to operate several times. In the regime of grain and source sizes treated here, the Hall-Petch relation has to be modified to include source effects. For small grains the source term dominates and one finds a flow stress dependence on the inverse film thickness (or grain size). The results indicate that the effect of dislocation sources has to be included into a theory of thin film plasticity.


Quantitative experimental observations of dislocation nucleation and glide in the model Al (011) / Si (100) thin film system are presented. Using a simple physical vapor deposition technique, a thin film composed solely of two symmetry-related grain orientations of (011) aluminum on Si (100) substrates can be created. This provides an ideal system within which to determine the specific behavior of dislocations during thermal stress relaxation. In prior work, it was shown that isoelectric transmission electron microscopy allows real-time observation of dislocation climb, cross-slip, grain boundary nucleation and glide. This paper was found that dislocation nucleation occurs preferentially at the cusp in the grain boundaries, beginning at a temperature of 275°C, followed by slip along the inclined (111) glide planes. Subsequent nucleation and glide along these same slip systems occurs sporadically upon further cooling, until the sample reaches a temperature of 75°C. At this point, dislocation nucleation and glide occurs instantaneously along all four n/2<110> (111) slip planes. Herein, we show the observation that this is a direct result of the anisotropy of stress in (011) oriented film. Anisotropic elasticity theory shows that the magnitude of the resolved shear stress on particular Burgers vectors of dislocations that lie on inclined (111) slip planes is substantially higher than on the perpendicular (111) slip planes for this (011) Al film. The calculations indicate that the stress on these dislocations at 275°C is on the order of 350 MPa. At a temperature of 75°C, the same analysis indicates a nearly identical level of stress on another set of dislocations that reside on both the inclined and the perpendicular slip planes, thereby directly explaining the experimental observations. These results indicate that the grain boundary nucleation of dislocations may play a critical role in the observed high strengths of metallic thin films on rigid substrates.

9:30 AM W3.4 INELASTIC DEFORMATION MECHANISMS IN POLYCRYSTALLINE TIN-LINE F.C. METALLIC THIN FILMS. Marco J. Kobylinski, Carl V. Thompson, MIT, Dept. of MS&E, Cambridge, MA; Mildred E. Gross, Bell Labs, Lucent Technologies, Murray Hill, NJ.

While the fine microstructure of polycrystalline metallic thin films is believed to be the origin of their high strength, a comprehensive understanding of the connection between strength and microstructure is still lacking. To explore the relations between strength and microstructure in a systematic manner, we performed a study employing submicron-thick Ag and Cu films on Si substrates, as well as submicron-size Cu interconnects (lines) on substrates. In particular, we will report on the effects that grain size, film thickness or line width, characteristic length of the dislocation entanglement, and temperature have on the flow stress of films and lines. We have found that the mechanical properties of the films and the lines are determined by two main inelastic mechanisms: diffusional creep and dislocation-mediated plasticity controlled by the thermally activated motion of dislocations through obstacles, which presumably are forest dislocations. As expected, diffusional creep is dominant at high temperatures and small grain sizes, while dislocation-mediated plasticity is dominant at low temperatures and large grain sizes. The transition temperature being a function of film thickness and average grain size. For diffusional creep, the relevant length scale is determined by the film thickness and average grain size, while in dislocation mediated plasticity, the relevant length is the average distance between the pinning points, which was found to be on the order of 50-100 nm. This value is substantially smaller than the average grain size, suggesting that dislocation-mediated plasticity is a process that determines the low temperature strength of the films. Finally, we have also found that the strength of the films increases with decreasing film thickness and grain size, but then reaches a maximum value with decreasing thickness and grain size. This behavior in the result of the interplay between dislocation-activated plasticity and dislocation climb.

10:15 AM W3.5 STRESS-DEPENDENT STRUCTURE OF 90° PARTIAL DISLOCATIONS IN Si. Karen Lin, D.C. Chrzan, Department of Physics, University of California, Berkeley, CA and Center for Advanced Materials, Ernest Orlando Lawrence Berkeley National Laboratory, Berkeley, CA. and Center for Advanced Materials, Ernest Orlando Lawrence Berkeley National Laboratory, Berkeley, CA.

The ability to predict the stable core structure of dislocations is an essential step toward predicting their mobility. Dislocation mobilities, in turn, influence the lower limit of strength. Ideally, core structure predictions should be constructed using an ab initio electronic structure total energy technique. This prediction is complicated, however, by the need to either study artificial arrangements of dislocations (i.e. periodic supercells), or by studying small, cylindrical systems while capping the dangling surface bonds. In the periodic supercell technique, the boundary conditions one imposes may exert a significant influence on the core structure of the dislocation. The use of periodic supercells for the prediction of the relative stability of the two proposed core structures for the 90° partial dislocation in Si (the so-called single-period and double-period core reconstructions) is explored. The total energies of a number of different cell configurations are computed using Tersoff potentials. It is demonstrated that 1) The periodic supercell technique produces results equivalent to those obtained by imposing cylindrical boundary conditions. 2) Tersoff potentials predict that the relative stability of the competing single period and double period core structures depends systematically on the applied shear stress. And 3) Tersoff potentials predict that pressure induces a transition in the stable core structure, with high pressure favoring the single-period core reconstruction. The support of the Director, Office of Energy Research, Office of Basic Energy Sciences, U. S. Department of Energy under contract No. DE-AC03-76SF00098 is gratefully acknowledged.

10:30 AM W3.6 ATOMIC SIMULATION OF KINK-PAIR ENERGY IMBALANCES OF SCREW DISLOCATIONS IN FCC IRON. Alfonso H. W. Ngai, Department of Mechanical Engineering, The University of Hong Kong, Hong Kong, PR CHINA; M. Wen, Advanced Materials Section, Production Fundamentals, Chaparral, National Industrial Research Institute, AIST, MITI, Hiroshima, JAPAN.

In bcc iron, there are two degenerate states A and B of the screw dislocation core. Motion of the screw dislocation core would hence proceed by jumps from A to B, B to A, etc. In this work, the nudged elastic band method is used to calculate the activation paths connecting such jumps. Kink-pairs are found to be involved in all such jumps. These kink-pairs are denoted according to the Duesbury scheme as BnApB, BnApA, BnApA and so on, where n and p denote the signs of the kinks, the first and third capital letters denote the state before jumping, and the middle capital letter denotes the state after jumping. Based on symmetry arguments, the set of possible kink-pairs is shown to reduce to only two non-equivalent heteroenergetic kink-pairs, BnApB and AnBpA, and one homoeotropic kink-pair, AnApA. The simulation results also show that the heteroenergetic kink-pair BnApB has significantly lower activation energy than the other heteroenergetic kink-pair AnBpA as well as the homoeotropic kink-pair AnApA. Hence, under a “negative” applied stress, the B to A jump is easy, but the A to B jump is difficult. The situation is reversed upon a “positive” applied stress. The difficult jump on the primary (111) plane can however be bypassed by jumping onto an intersecting cross-slip plane, the morphology of which is easy to the jump on the primary plane. The motion of the screw core would therefore be zigzagging and the average slip plane would tend towards the mirror plane. We believe this is the proper explanation of the observed pencil glide at elevated temperatures. The activation energy of the nano-controlling BnApB kink-pair depends on the applied stress, and the activation energy is the limiting process at a critical event appears to be the transmission of dislocations across interfaces. At larger layer thickness, deformation occurs by confined layer slip within individual layers, followed by slip by slip by slip. This mechanism monotonically increases with decreasing layer thickness. As smaller layer thickness, the stress for confined layer slip becomes so large that
The first observations of Chokshi et al. (1) of softening with decreasing grain size for nanocrystalline Cu and Pd stimulated interest in this apparent inverse Hall-Petch behavior for decreasing grain size in the nanoscale regime. However, it was subsequently pointed out that for most of the experiments where inverse Hall-Petch behavior was observed, the grain size was beyond the initially finest grain size specimens to grow the grains. It was suggested that thermally treating nanocrystalline samples may cause changes in the structure (e.g., decreases in porosity, changes in grain boundary structure, etc.) along with the grain growth and the changes may be responsible for the inverse Hall-Petch behavior. In spite of the uncertainty in the experimental evidence for the inverse Hall-Petch effect, a number of mechanisms have been proposed to explain its occurrence. Molecular dynamics simulations have also predicted the inverse Hall-Petch effect. Since conventional dislocation-induced deformation mechanisms are unlikely at the finest nanocrystal grain sizes, changes in the dislocation density dependence of hardness and strength are more surprising. This paper will critically review the available experimental evidence for the inverse Hall-Petch effect and discuss it in the context of the simulation studies and the various proposed mechanistic models.


Support from NSF under grant no. DMR-9871980.

2:00 PM W4.2/B5.2

LARGE TENSILE DUCTILITIES AND ULTRAHIGH YIELD STRENGTHS AT ROOM TEMPERATURE IN NANOCHIPS.

TALLINE Fe-Co ALLOYS. Chang He Shang, D. Van Heerden, R.C. Chambers, The Johns Hopkins University, Department of MS&E, M.C. Chien, The Johns Hopkins University, Department of Physics and Astronomy, Baltimore, MD; T.P. Weihs, The Johns Hopkins University, Department of MS&E, Baltimore, MD.

Researchers have pursued nanocrystalline materials for structural applications for more than a decade because materials with grain sizes below 1 micrometer have been predicted to display and, in some cases, have shown significant improvements in mechanical properties compared to coarse-grained materials. High yield strengths and superplasticity have been demonstrated, and enhanced ductility has been predicted for nanocrystalline intermetallics. However, while nanocrystalline Cu has shown enhanced ductility at room temperature, nanocrystalline intermetallics typically fail in the elastic regime with less than 1% strain-to-failure. The extreme brittleness in nanocrystalline intermetallics is generally attributed to flaws or porosity that are produced during fabrication. In this study, we have investigated the mechanical properties and microstructures of fully dense, single-phase nanocrystalline Fe-Co alloys that were fabricated using bulk processing techniques. The nanostructured alloys possess very attractive mechanical properties at room temperature with tensile yield strengths as high as 2.2 GPa and tensile ductilities ranging from 3% to 18%. Both tensile strengths and hardnesses follow Hall-Petch relationships, and the fracture surfaces show ductile features. Results from TEM, SEM, and X-ray diffraction investigations will be used to understand the microstructure of these flaw-free, nanocrystalline materials.

2:15 PM W4.3/B5.3


1Dept. of MS&E, Johns Hopkins Univ., Baltimore, MD.

Full density Fe with grain sizes in the nanophase to submicron range has been consolidated from mechanically milled powders. The deformation behavior of such materials, as a function of grain size, strain rate, and temperature, have been studied using quasi-static and high strain rate (Kolsky bar) tests. With ultradense grain sizes, Fe exhibits high strength, little work hardening, and plastic strains localized in shear bands. Shear banding appears to be the dominant mode from the onset of the plastic deformation in our consolidated materials. Little strain rate sensitivity of the flow stress is observed over a wide strain rate range (up to 500s-1). These behaviors are contrasted with those of conventional bulk Fe, which shows uniform deformation, significant work hardening, and strong strain rate sensitivity. The underlying deformation and failure mechanisms are discussed based on these observations. With increasing strain rates and higher temperatures, the yield stress increases and prior deformation strain increases. These findings are compared with the Hall-Petch relationship, and examined to determine the validity range, in terms of grain size, temperature, strain rate, and particle bonding strength, of different deformation mechanisms (e.g., dislocation climb, grain boundary mechanisms). In addition, we comment on the potential advantage of related bulk alloys in military kinetic energy penetrators where the shear banding mode and self-sharpening capability during high-rate deformation are desired.
Mechanical Milling (MM) using a high energy ball mill was applied to iron powder to obtain ultrafine-grained structure. The MM treatment causes a marked increase in the hardness of iron powder from HV0.2 to 800 GPa. Initial hardness in MM is due to well-known dislocation strengthening, but the latter hardening (above HV0.2 GPa) is mainly due to grain refining strengthening. The grain size of iron powder with the hardness HV0.2 was about 250 μm. In the Hall-Petch plot of the initial ultrafine-grained iron, a linear Hall-Petch relationship was confirmed to occur around 10 μm but the plots below 100 nm in the grain size deviated toward lower hardness side from the extended Hall-Petch line. In a 0.85% C powder, grain size was refined to 10 μm but the hardness was also much smaller than the value expected by the extended Hall-Petch line and showed a tendency of levelling-off at HV0.2 GPa. As a result, the grain size of iron is seen to be refined to around 10 μm by severe deformation and the hardness achieved by grain refining is thought to be about HV0.2 GPa (expected yield strength: 3.6 GPa).

ATOMIC STUDIES OF PLASTICITY IN NANOPHASE METALS. S. A. Caro, Centro Atómico Bariloche, Bariloche, ARGENTINA; T. Van Swygenhoven, P. Derlet, Paul Scherrer Institute, Villigen, SWITZERLAND; D. Park, Dept. of MSE, Virginia Polytechnic Institute & State Univ., Blacksburg, VA; M.J. Caturra and T. Diaz de la Rubia, Lawrence Livermore Nat. Lab., Livermore, CA.

We have studied structural, energetic, elastic, and plastic properties of a family of computer-generated nanoparticle samples of Cu and Ni, continuously increasing the average grain size, covering now the range from 20 to 3.5 nm. Properties that can directly be compared to experiments, like density, excess enthalpy, and elastic constants, show a remarkable agreement suggesting that the computer modeled materials are able to capture the essential features of the real nanoparticle metals. Investigating the structure of the grain boundaries on the atomic level, we found that the grain boundaries in nanoparticle metals are essentially similar to those found at the macro scale, i.e., similar structural units are found, providing evidence against the view of grain boundaries in nano-crystallites as amorphous or liquid-like interfaces. One of the most striking features is the observation of a change in plastic regime as the grain size approaches the ~10 nm region. In fact, intragrain dislocation activity ceases to operate below this size and grain boundary sliding, a process based on mechanical and thermally activated single atomic jumps, dominates the contribution to deformation. It in turn implies that deformation becomes easier as the grain size further decreases. This observation is of primary importance in the interpretation of the inverse Hall-Petch relation reported experimentally. The computer simulations provide access to a microscopic view of the deformation processes. In this way we obtain a detailed description of the structure and energetics of grain boundaries and triple junctions, identifying the regions where dislocations are generated when the grain size is large enough, as well as the mechanism on atomic level of grain boundary sliding. We extract quantitative information about the conditions for dislocation emission and the role of the atomic structure of the grain boundaries.

GRAIN-BOUNDARY CONTROLLED DEFORMATION OF NANOCRYSTALLINE MATERIALS BY MOLECULAR-DYNAMICS SIMULATION Dietzel-Wolf. Materials Science Division, Argonne National Laboratory, Argonne, IL.

Molecular-dynamics (MD) simulations of model nanocrystalline microstructures demonstrate that the high-temperature plastic deformation process involves grain-boundary diffusion creep. In order to suppress grain growth and thus to enable steady-state deformation to be observed on a time scale accessible to MD simulations (typically 10^4 s), our input microstructures were tailored at (i) have a uniform grain shape and a uniform grain size of up to about 10 nm and (ii) contain only high-energy grain boundaries which are known to exhibit rather fast, liquid-like self-diffusion. Our simulation setup is to study the time-dependent diffusion process with a degree of homogeneity (i.e., involving no grain sliding), with a strain rate that agrees quantitatively with that given by the Coble-creep formula. The extension of these results to lower temperatures, with emphasis on the comparison to the experimental data, is currently in progress. Work supported by the U.S. Department of Energy, Office of Science, under Contract W-31-109-Eng.38.

GRANITE MICROSTRUCTURE EVOLUTION IN NANOSCALE MATERIALS - RECENT SIMULATION RESULTS. Moneesh Ugrumov et al. 1,2 and David J. Srolovitz 1,2, 3 Princeton Materials Institute, Princeton, Princeton University, NJ; 2Dept. of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ; 3Dept. of MSEE, University of Michigan, Ann Arbor, MI.

The mechanical properties of many materials vary with grain size. For example, the yield strength varies with grain size as in the well-known Hall-Petch relation and creep properties vary with grain size in Coble creep. Such effects are especially important on the nano-scale. In this study, we examined several issues associated with the evolution of the grain structure. In particular, we study several important issues in grain size evolution that only become important when the grain size is very small. These studies were performed using molecular dynamics simulations in two- and three-dimensions. We examine the range of grain sizes over which the classical concepts of grain boundary mobility and curvature driven growth apply and the effects of grain boundary triple junctions and grain rotation on grain boundary migration. These latter effects are commonly neglected in models for grain microstructure evolution. The present results suggest that the boundary velocity is proportional to boundary curvature, at large grain sizes, but increases superlinearly with decreasing grain sizes at very small grain sizes. We have also explicitly extracted grain boundary triple junction mobilities for a large number of grain boundary martensitic transformations. We find that while the triple junctions provide a drag on boundary motion, this drag is negligible at all grain sizes (down to a couple of nanometers). However, we have identified several strain microstructures where the triple junction mobility is low enough to significantly slow boundary migration. Finally, simulations of shrinking grains demonstrate that at sufficiently small size, grains rotate as they shrink. Interestingly, this rotation is not completely consistent with expectations based on the orientation dependence of the boundary energy and does not require the motion of lattice dislocations.

THE HALL-PETCH RELATION IN NANOCRYSTALLINE METALS. J. Schiats, Center for Atomic-Scale Materials Physics and Department of Physics, Technical University of Denmark, Kongens Lyngby, DENMARK.

It has not yet been settled to what extent nanocrystalline metals obey the Hall-Petch relation, i.e., whether the yield stress and hardness increase with decreasing grain size. There are conflicting experimental data concerning a possible reverse Hall-Petch effect, a softening with decreasing grain size at the smallest grain sizes. The experimental ambiguities are probably caused by the extreme difficulty of manufacturing samples of sufficient quality. We have previously used atomistic-scale simulations to demonstrate that nanocrystalline copper and palladium with grain sizes below 13 nm exhibit a reverse Hall-Petch effect, caused by sliding in the grain boundaries [Schiats et al., Nature 361, 561 (1993); Phys. Rev. B 60, 11971 (1999)]. Based on these simulations, a model is presented that attempts to give a unified description of the yield stress of polycrystalline metals for all grain sizes. The model is based on a competition between two deformation mechanisms: activation of dislocation sources in the grains and grain boundaries, and grain boundary sliding.

SESSION W5: POSTER SESSION

Wednesday, November 28, 2000
8:00 PM
Exhibition Hall D (Hynes)

W5.1 HARDNESS OF SEMICONDUCTORS. Ichiro Yoshino, Tetsuya Hoshia, Institute for Materials Research, Tohoku University, Sendai, JAPAN.

Hardness of various semiconductors such as Si, Ge, InSb, ZnSe, GaN, GeSi alloys, etc. was surveyed in a wide temperature range from RT to close to the melting point of the material. The Vickers indentation hardness of (111) surfaces of the crystals of diamond-type and sphalerite-type, shows a typical temperature dependence: a gradual decrease from RT to intermediate temperatures, then steep decrease with increase of the temperature. The hardness of (111) surfaces of SiC shows a steep decrease at high temperatures following a plateau in the intermediate temperature range. The temperature dependence of the hardness is expressed by a universal relationship H_v = HRT / (1 + AT)^n, where H is the shear modulus and n the magnitude of the Burgers vector. The steep decrease of H_v at elevated temperatures can be described by the phenomenological relationship H_v = HRTexp(U/kT). The estimated
value $U$ for various semiconductors is proportional to the activation energy of dislocation motion previously reported for these crystals.

W5.2 THERMALLY-ACTIVATED INITIATION OF PLASTICITY IN SILICON. N. Yang and Y.Q. Sun, Department of MSE, University of Illinois, Urbana, IL.

Thermally activated plastic deformation in single crystal Si is studied. Samples oriented for single slip are loaded by a dead-weight load or shear until the critical temperature is increased through the point of brittle-to-ductile transition. The initiation of plastic deformation at the critical temperature, in particular the initial transient plastic strain-rate, is investigated using a high-resolution displacement sensor with a fast data-acquisition rate. Particular attention is given to the extent of plastic strain localization and the local strain-rates. The transition temperature is measured against the stress. The relation found between stress and the critical temperature is used to estimate the thermal activation parameters. The results are compared with plasticity initiation models based on dislocation nucleation and multiplication.

W5.3 ON THE EFFECTIVE TENSILE STRENGTH OF LIQUIDS UNDER DYNAMIC STRESSING: THEORY AND EXPERIMENT. P. Rhode Williams, Stephen W.J. Brown, Rhodri L. Williams, University of Wales-Swansea, Centre for Complex Fluids Processing, Dept. of Chemical and Biological Process Engineering, Swansea, UNITED KINGDOM.

We consider some discrepancies arising between different measurements of the effective tensile strength of liquids under dynamic stressing, in experiments involving the creation of negative pressure with the relaxation of the pressure pulse at a free surface. We critically examine the structure of the pressure records reported in such experiments and conclude that a key feature of many of them may have been misinterpreted in previous work. A complete explanation of such pressure records is presented here: this explanation suggests a hitherto unsuspected mechanism for the order of magnitude discrepancies in dynamic tension recorded in previous dynamic stressing experiments. We present a new method of estimating the effective tensile strength of liquids under an explosion procedure in the range of static positive pressures. This method, which provides an estimate of the maximum dynamic negative pressure sustained by a liquid, differs from previous techniques which have involved long extrapolations into the negative pressure regime. The results obtained indicate that denatured water can sustain a transient tension of nearly 300 bars, reordering the results of pulse reflection work with those of other dynamic stressing techniques. Results are also reported for other liquids, including dilute solutions of high molecular weight polymers, liquid mercury and multigrade motor lubricants at elevated temperatures.

W5.4 MOLECULAR-DYNAMICS STUDY OF INSTABILITIES IN CRYSTALS UNDER CONSTANT STRESS. Jianhui Zhao, Frederick Milstein and Dimitris Merakos, Univ. of California, Santa Barbara, CA.

Mechanical, geometric, and kinetic characteristics of crystal instabilities are revealed via non-crystal molecular-dynamics (MD) simulations according to the Lagrangian formulation of Parrinello and Rahman. Results are analyzed in terms of the elastic stability criteria of Hill and Miekle. Fluctuation formulae are used for computation of elastic moduli employed in measurements of elastic stability. Intramolecular interactions in metals are expressed both by simple Morse pair potentials and by more accurate semi-empirical embedded-atom-method potentials that have been parameterized specifically for studies of crystal elasticity at finite strain. As an example, the stability of bulk crystals was studied under constant pressure and temperature. It was found that violations of the elastic stability criteria predict the onset of bcc-to-hcp transitions. Computations were carried out on the crystals’ shear moduli at each pressure and temperature and of the evolution of the crystals’ enthalpies along the transformation paths. Under isothermal-isobaric conditions, the bcc-to-hcp transitions proceeded according to the Burgers mechanism. Most importantly, the transitions were found to occur at the minimum of the pressure potential at an elastic instability that is associated with vanishing or diminishing shear moduli.

W5.5 Abstract Withdrawn.

W5.6 FIRST-PRINCIPLES STUDY OF THE STRENGTH AND FRACTURE OF GRAIN BOUNDARIES IN SILICON CARBIDE. Mamoru Kobayashi, Dept. of Materials Physics, Osaka National Research Institute, Ikeda, Osaka, JAPAN.

It is of great importance to understand the mechanical properties of SiC grain boundaries, which seriously affects bulk ceramic properties. First of all, it is essential to clarify the behavior of grain boundaries under various tensile or shear stresses. Currently, first-principles calculations using the pseudopotential method based on the density-functional theory can be applied to such complex problems. We have performed the ab initio tensile tests of a coincidence tilt boundary in cubic SiC. The same energy change to the boundary is examined first. These interfaces have the same bonding network, although the polar ones contain either C-C or Si-Si strong bonds and the non-polar one contains both kinds of strong bonds. In the tensile test, the stress is controlled by a small increment, and all the atoms are relaxed. This cycle is iterated until the interfaces are broken. This corresponds to a real tensile test at T<Elk. Young’s modulus, tensile strength, fracture energy, and fracture toughness are obtained for these interfaces. Features of fracture, bond breaking and changes in the electronic structure are analysed in detail. Results of each interface are compared with each other and with bulk SiC. We discuss the effects of C-C and Si-Si strong bonds on the tensile strength and fracture, and the effects of temperature and impurities.


Amorphous-Diamond (a-D) thin films deposited by pulsed-laser deposition typically have high levels (6-10 GPa) of residual stress. This stress is thought to be intrinsic to the deposition process, but is not intrinsic to hard (> 85 GPa) a-D films, since thermal annealing to moderate temperatures (600°C) can completely remove the stress without significantly changing the 4-fold carbon content. We have taken advantage of these low stress a-D films to create true surface micromechanical structures [cantilever beams, tensile pull tabs, notched beam pull tabs, and friction test structures] to evaluate the micromechanical properties of these films. For example, early tensile test results done with a non-indenter show that the 4-D fracture strength is quite high, > 8 GPa, much higher than CVD diamond films (~1 GPa) which tend to be highly defective. In addition, cantilever beam bending experiments show that the modulus of this material is also quite high (> 700 GPa) and does not change significantly with annealing to 950°C. Human analysis of the annealed a-D films show that the character of the 3-fold carbon bonds change with annealing while EELS on plan-view samples indicates almost no change in the 3-fold content. We are in the process of making spatially resolved EELS measurements on cross-sectioned samples of annealed a-D to investigate the bonding content while keeping the same enhanced mechanical properties reported above for these films. In addition, we have prepared samples with enriched 13C for NMR analysis. This work was supported by the U.S. DOE under contract DE-AC04-94AL85000 through the Laboratory Directed Research and Development Program, Sandia National Laboratories.

W5.8 FAILURE OF ELECTRODEPOSITED METALLIC NANO-STRUCTURES. Ferenczek Erbom, MSE Dept., University of Florida, Gainesville, FL.

We have fabricated nanocylindrical and nanocrystalline samples of FCC metals via electrodeposition techniques. The properties of these nanostructures are characterized using x-ray diffraction, transmission electron microscopy, scanning electron microscopy, microcalorimetry, and tensile testing techniques. The single-phase nanostructures failed in a ductile manner when the fabricated material did not have weakened paths such as grain boundaries with high concentrations of impurities or intergranular boundaries. Excessive co-deposition of hydrogen resulted in formation of ultrafine voids, which led to microvoid coalescence fracture mechanism. Otherwise, all electrodeposited single-phase FCC nanocrystals fracture by the so-called knife-edge mechanism. The limit strength of these materials will be discussed in terms of work hardening and plastic instability. The laminated nanostructures consisting of two different metallic layers with FCC crystal structures, however, showed cleavage-like fracture. One explanation is that local stresses as high as the theoretical strength develop in nanocomposites materials. The other possibility is that deformation at interfaces or a high density of processing voids provide the opportunity for tensile of ultrafine ligaments, which look like cleavage facets. The possibilities of these mechanisms are discussed in Cu/Ag and Cu/Al electroplated structures.
W5.9 THE EVALUATION OF ELASTIC MODULUS AND ADHESION ENERGY OF DIAMOND-LIKE CARBON FILM WITH ENERGY METHOD, Myung-Woo Moon, Kyu Hwan Oh, School of MSE, Seoul National Univ., Seoul, KOREA, JunWon Chung, Kwang-Ryoo Lee, Thin Films, Optoelectronics Research, Korea Institute of Science and Technology, Seoul, KOREA.

This study presented a new evaluation method of fundamental adhesion energy and elastic modulus of diamond-like carbon (DLC) film under highly compressive stress state which caused the elastic instability, buckling. The analysis was executed by experiment and theory for DLC film deposited by CVD. To estimate these two elastic properties with adhesion devices or on artificial surfaces, the residual stress of buckling on the same specimens could be established. The one was the buckling buckling which was self-hardened phenomenon, and the other was the free buckling which could be developed with artificial technology instead of the side of delaminated film suggested by K.-R. Lee et al. With analysis of buckling, simple equation for adhesion energy and elastic moduli were taken into account independently with energy method which energy balance could be equivalent between before and after buckling. The adhesion energy at the interface between film and substrate needed to be considered in analysis of delaminating buckling, but not to be considered in analysis of free buckling because of no interface adhesion which was removed by substrate etched. The free buckling could be developed by artificial technology which was the anisotropic etching Si substrate only cut. And we could make the edge of DLC overhanging free from contact of Si substrate. The compressive stress due to deposited in deposition process could be released as the form of the sinusoidal buckled wave. And this wave could be experimentally observed as well-developed wavelength and amplitude in etched film and known as in deposition conditions that affected the elastic properties of film. From experimental data and analytic equation for free buckling, the elastic modulus could be easily calculated and were evaluated from 70GPa to 280GPa for DLC films in stress changes from 0.6GPa to 2.1GPa. The adhesion energy could be evaluated by the analysis of buckled geometries of delaminating buckling, and in this analysis the calculated elastic modulus of DLC film in the analysis of free buckling could be used due to some specimen. Then the fundamental adhesion energy of DLC film on Si substrate could be evaluated such that the range from 0.39 Nm to 1.17 Nm with increasing stress of film from 0.6GPa to 2.1GPa proportionally. In summary, the free buckling could be developed at the side of delaminating buckled film by substrate etched. By free buckling the elastic modulus could be estimated, and the fundamental adhesion energy of thin film could be calculated without no other device by combining with the analysis of delaminating buckling and the calculated elastic modulus.

W5.10 HYDROGEN INDUCED MULTI-VACANCY FORMATION IN HYDROGEN EMBRITTLEMENT OF α-Fe, Yoshito Kato, Takahisa Ohno, Natl. Res. Inst. for Metals, Tsukuba, JAPAN.

Hydrogen effects on void formation at the initial stage of fracture and during crack propagation has been one of the important problems of hydrogen embrittlement of iron-based structural materials. Several effects related with lattice cohesion or dislocation have been already proposed, whereas they are not conclusive yet. Recently, some forms of micro-hydrogen generation from macro-hydrogen complexes have also been reported. In this work, we focus on this vacancy-hydrogen system in pure α-Fe and present hydrogen effects on the multi-vacancy formation investigated by first-principles supercell simulations. Concerning the stability of monovacancy, we found that monovacancy is most stabilized by trapping two H atoms inside at ambient condition. This complex VacH2 leads to about 30% reduction of the monovacancy formation energy due to the hydrogen bonding. H2 is the 3rd bonding of VacH2. On the other hand, the VacH4, which has been believed to be the most stable, is found to be energetically unreachable to the monovacancy without H. These results provide a new insight for the vacancy clusterization mechanism. This VacH4 is the more clustering is expected to be unfavorable due to the decrease of H sites in the vacancy cluster and the occupation of interstitial sites with higher energy by surplus H. On the other hand, this situation does not occur in the case of VacH2, suggesting that the multi-vacancy formation is favorable. The present study clarifies that hydrogen can largely affect the void formation through the vacancy formation and clusterization. By comparing the lattice decohesion mechanism with the present results and considering the competition between vacancies and dislocation motions, we discuss possible mechanisms for the hydrogen embrittlement of α-Fe.


Plasticity in thin films has been extensively studied by macroscopic nanoindentation techniques such as micro-cantilever testing, microindentation, and conventional x-ray diffraction, but is still not fully understood. In the present work, we have investigated the plastic phenomena by using Microbeam X-Ray Diffraction (μXRD) combined with macroscopic thin film mechanical test. This technique is able to resolve the full strain/ stress tensor (6 components) and texture (orientation matrix) at submicron scale in thin films with an accuracy of 2° in strain and less than 0.1° in orientation. In contrast to the complementary technique of CED (Convergent Beam Electron Diffraction) in Transmission Electron Microscopy, no sample preparation is necessary (i.e. the strain/stress state remains unaltered). Local plastic deformation of single grains in sputtered Cu blanket films (0.13 - 1.5um thick) was studied between room temperature and 220°C. Furthermore, we measured effects of two-dimensional confinement of passivated Al lines (0.7um wide) and passivated and unpassivated electroplated Cu damascene lines (0.8 to 5um wide) at temperature varying from room temperature to 300°C. The results indicate noticeable strain and texture variations within individual single grains.

W5.12 DETERMINATION OF STRESS ORIENTATION DISTRIBUTION FUNCTION IN POLYCRYSTALLINE MATERIALS WITH NEUTRON DIFFRACTION. Yau-Chang Wang and Xin-Li Wang, Spallation Neutron Source Project, Oak Ridge National Laboratory, Oak Ridge, TN.

The stress or strain incompatibility between grains having different crystallographic orientations can lead to grain orientation-dependent stress heterogeneity, generally known as the intergranular or type II stress. The appearance of this intergranular stress has severely compromised our ability to specify actual stress levels in the engineering component under examination. It is now generally understood that this incompatibility is mainly caused by the stress anisotropy of elastic or plastic behaviors in single crystals. Therefore, determination of the intergranular stress will not only allow us to deduce the macroscopic (or engineering) stress in a component with much more confidence, but also shed light on the fundamental mechanism of grain-to-grain interactions during elastic and plastic deformations. Recently, a new concept called stress orientation distribution function (SOD) was introduced to describe the intergranular stress in polycrystalline materials. Similar to the crystal orientation distribution function (CODF), which is used to quantitatively describe crystallographic texture, SODF describes the microfield stress as a function of the grain orientation, or stress texture. In contrast to previous works that rely on numerical modelling of a specific thermomechanical process, SODF provides an experimental means to characterise the intergranular stress heterogeneity. Stated differently, it is possible to determine the stress anisotropy of materials where the prior deformation history is unknown, the intergranular stress heterogeneity can still be described in a quantitative manner. In this paper, recent progress in determining SODF from neutron diffraction measurement results is presented.

W5.13 INTERFACIAL STRENGTH AND FRACTURE AT Au/Al2O3 INTERFACE. S.X. Xu, Department of Mechanical Engineering, University of Pittsburgh, Pittsburgh, PA.

Interfacial strength and fracture at Au/Al2O3 interface in layered materials are investigated for the first time in this work. Fracture testing has been carried out to measure the interfacial strength and toughness using Al2O3/Au/Al2O3 sample. The associated interfacial strength of Au/Al2O3 is crack tip has been found to be 14 GPa and 3 GPa in dry and moist air environments by measuring the critical crack tip blunting distance using atomic force microscopy. Modelling on the interfacial strength and fracture toughness has been carried out. The dislocation plasticity in the metal layer is considered, and the net energy for initial emission of a dislocation is assumed to be attained before the cleavage of the interface crack. Superdiffusion modeling is employed to obtain the critical strain energy release rate, for interface separation from crack tip. When a stress separation based on surface stress at the interface crack tip, interface debonding occurs and the crack propagates. This model predicts the strong dependence of interfacial fracture toughness on the interfacial strength under mixture of normal and shear loading.
SESSION W6/Q: JOINT SESSION
LIMITS OF STRENGTH IN INDENTATION
Chair: Murray S. Dow and Jocot J. Vrielinck
Thursday Morning, November 30, 2000
Room 309 (Hynes)

8:30 AM W6.1/Q.1
EXPERIMENTS ON THEORETICAL STRENGTH AND SIZE EFFECTS IN INDENTATION: P. D. Nix, Rozijn's Suh, Eric T. LilleILED, David Barbero and Bruce M. Clemens, Department of MSE, Stanford University, Stanford, CA.

Nanoindentation permits the study of plasticity of materials in very small volumes, from the atomic and molecular scale, through the mesoscopic scale to the continuum scale. As such, it provides a particularly good tool for validating the predictions of multiscaling modeling and simulations of material behavior. Various plasticity experiments at small length scales will be described. Here we consider individual Dislocation Effects, involving the nucleation of dislocations in perfect crystals and Multiple Dislocation Effects, as revealed by various indentation size effects. Nanoindentation of Mo and its epitaxial films and Au single crystals at the nanometer depth scale reveals irregular load-displacement curves that appear to be associated with the nucleation of dislocations. The contact pressures at which the first inelastic events are triggered compare favorably with recent calculations of nanometer scale indentations in perfect crystals. We show that these discrete plastic events are strongly affected by the proximity of high-angle grain boundaries, suggesting that grain boundaries can play a role in dislocation nucleation. We have shown that the indentation size effect on hardness of crystalline materials can be accurately modeled using the concept of geometrically necessary dislocations and that this can be used to formulate a law for strain gradients in indentation. Here we describe a new type of nanoindentation experiment to show the effect strain gradients on flow strength. A strong plastic strain gradient is created by indenting a soft film on a hard substrate with a sharp diamond indenter. The hardness of the film is observed to increase with increasing depth of indentation, in sharp contrast to the falling hardness with increasing depth in bulk materials. We attribute this rise in hardness with the strong gradient of plastic strain created between the indenter and the substrate to the model calculated using a recently developed model of strain gradient plasticity.

9:00 AM W6.2/Q.2
CONNECTING ATOMIC AND EXPERIMENTAL ESTIMATES OF IDEAL STRENGTH, C. R. Kreen 1, 2, D. Roundy 1, 2, Mervin L. Cohen 1, 2, D. C. Chrzan 1, 3, and J. W. Morris Jr. 1, 3, 1 University of California at Berkeley, Dept. of Materials Science and Engineering, 2 University of California at Berkeley, Dept. of Physics, 3 Lawrence Berkeley National Laboratory, Materials Sciences Division

Using ab initio techniques, it is now possible to calculate the ideal shear strength in crystals with considerable accuracy. However, nanoin indentation techniques are also possible to experimentally apply stress levels of the order of the ideal shear strength to defect-free regions of high purity single crystals. However, realistic determination of the stress fields produced by high stress nanoin indentation requires finite element modeling. We use a finite element model incorporating a nonlinear stress-strain curve of the same form as that calculated ab initio for bcc tungsten to determine the maximum shear stresses reached beneath a sharp spherical indenter on a nonlinear elastic substrate. This model yields a load-displacement curve very similar to the Herzig linear-elastic solution, but the peak shear stresses beneath the indenter are only 70% of those obtained from the Herzig solution. We use the results of this study to compare ab initio ideal strengths with the maximum shear stress reached during nanoin indentation of tungsten and molybdenum by Nix et al. and Gerberich et al. and find very good agreement. We conclude that the upper limit of strength during nanoin indentation is set initially by the shear stress in the initial defect-free tungsten and molybdenum is governed by the limits of elastic stability and suggest that other materials may behave similarly.

9:15 AM W6.3/Q.3
THE ROLE OF MICROSTRUCTURAL LENGTH SCALE IN INDENTATION BEHAVIOR OF GOLD, Erica T. Lille-leden, William D. Nix, Stanford University, Dept. of MSE, Stanford, CA.

Observations of depth dependent hardness have been made for various metals, and have been well described, in part, by strain gradient constitutive laws. However, strain gradient models maintain a continuum framework and cannot be expected to explain discrete load-displacement behavior widely observed at the nanometer scale. Such observations of discontinuities in the initial stages of indentation imply that dislocation nucleation occurs, in agreement with atomistic calculations. However, the two descriptions, strain gradient analyses and dislocation nucleation considerations, rely on opposing limits of the relation between dislocation density and strength, implying a critical discrepancy between these models. Here, we present experimental evidence of indentation size effects in hardness for gold thin films of various thicknesses. The observations are described in terms of dislocation nucleation and activation, and classical relations between the indentation size effects are reviewed. We find that the grain size affects both the critical loads for the onset of dislocation activity and the evolution of hardness with indentation depth. In particular, a Hall-Petch type strengthening mechanism is shown to play a substantial role in the indentation size effects of small-grained films, overwhelming the strain gradient effects. Additionally, the competition between dislocation nucleation and activation of pre-existing dislocations is related to the grain structure and the proximity of the indentation to the grain boundary.

9:30 AM W6.4/Q.4
PHYSICAL ORIGIN OF A SIZE EFFECT IN NANO-INDENTATION, A. J. Bushby 1, J. R. Downes 1, N. J. Gnjewska 1, 2, P. Kidd 3, A. Kelly 3, and D. J. Whelan 3, 1 Department of Materials, 2 Department of Physics, Queen Mary and Westfield College, University of London, UNITED KINGDOM, 3 Dept of Math Sci & Metallurgy, Univ. of Cambridge, UNITED KINGDOM

We have reported results of nanoindentation using spherical indenters to observe the full stress-strain curve. We observe the onset of plasticity in semiconductor strained-layer superlattices. These structures have alternating layers of two materials, each containing a covalent bond. The yield point is reduced by the presence of the coherency strain. By varying the thicknesses and strains, we have been able to show that both sets of layers, compressive and tensile, reduce the yield point. This suggests that a yield criterion must be satisfied over a finite volume, large enough to include layers of both signs. In these studies, we have observed a large and reproducible size effect in the yield point. That is, with smaller radius indenters, the mean pressure over the contact area is lower than that of purely elastic behavior increases, by up to a factor of two for a 2 micron radius indenter tip. Here we show how the requirement of meeting a yield criterion over a finite volume naturally leads to the size effect. Essentially, with small radius indenters, the peak stresses must be greater in order to achieve a given average stress over a finite volume. A theoretical analysis is given and quantitative agreement with experiments is obtained. This is consistent with our understanding of nanoindentation and other systems in which stresses are highly inhomogeneous on a small scale.

9:45 AM W6.5/Q.5
IN-SITU NANINDENTATION OF TRANSITION METAL CARBONITRIDES IN A TRANSMISSION ELECTRON MICROSCOPE, A. M. Minor, Department of MSE, University of California, Berkeley, CA and Center for Advanced Materials, Lawrence Berkeley National Laboratory, Berkeley, CA; E. A. Sched, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA; C. R. Kreen, J. W. Morris, Jr., Department of MSE, University of California, Berkeley, CA and Center for Advanced Materials, Lawrence Berkeley National Laboratory, Berkeley, CA.

The mechanisms of nanomechanical deformation in ultrahard materials such as the transition metal carbides are poorly understood. We have recently developed a nanoindentation TEM specimen holder which gives us the ability to make real-time observations into the nanomechanical response of various materials. We will show results from real-time nanoindentations of transition metal carbides and the subsequent analysis of the resulting indentation damage. Our results will be compared to prior ex-situ indentations of ultrahard materials, and to ongoing theoretical calculations of the ideal strength of these materials. We will also discuss issues related to the experimental procedures, including the unique specimen geometry required for the in-situ nanoindentations and the effects of the thin film on the indentation.
nanoproperties and diamond surfaces: the wear processes responsible for diamond polishing, and the mechanical deformation of tip and surface during indentation of the Surface Morphology (CM-AFM). The strong asymmetry in the rate of polishing between different directions on the diamond [110] surface is explained in terms of an atomistic mechanism for nano-machining processes. Although the direct observation is still out of reach, the process can be studied in two steps. Separate simulations in which a rigid tip was incident from the soft and the hard polishing directions on a single nanoasperity show pronounced differences in the indentation response. Then these differences inasperity removal are related to the process of nanogrooving by changing the boundary conditions at the edge of theasperity to recreate an ideal surface. The post-polishing surface morphology and the nature of the polishing residue predicted by this mechanism are consistent with experimental evidence. In the case of CM-AFM, it is shown that it is possible to tip terminated in a single atom to measure the data in coincidence. The magnitude of the normal force was unexpectedly found to be very similar for the approach on top of an atom or on a hollow position on the surface. This behavior is due to tip-relaxations induced by the interaction with the surface. These forces are also rather insensitive to the chemical nature of the tip apex.

10:45 AM W6.7/8.7

SINGLE CRYSTAL INDENTATION: OXIDE RUPTURE, SURFACE ASPERITIES AND THE YIELD POINT PROCESS. Donald E. Kramer, Natl Inst of Standards & Tech, Gaithersburg, MD; Karl B. Yoder and William W. Gerberich, Univ. of Minnesota, Dept. of Chemical Eng & Math Sci, Minneapolis, MN.

Nanoindentation of metallic single crystals has been a topic of recent investigations. This is a result of their ability to withstand near theoretical contact without showing signs of plastic deformation. When plasticity occurs, it manifests itself as a yield point, a sudden discontinuous increase in indentor displacement and a decrease in contact pressure. It has been suggested that dislocation nucleation is the time dependent plastic deformation mechanism for the time dependent and instantaneous injection of plasticity under these conditions, while the importance of an oxide or contamination layer has been retrospectively unexplored. This study combines atomic force microscopy (AFM) with nanoindentation to demonstrate the roles that oxide films and asperities play in the yield point process. Time dependent and instantaneous yield point properties were investigated for single crystals of tungsten and Fe 3%-Si. AFM observations indicate that the presence of asperities has a dramatic effect on the time dependent yield point properties. Measurements on the dependence of yield point load on oxide film thickness are used to develop a fracture mechanics based model in which oxide film fracture controls the yield point process. The results suggest that dislocation nucleation can occur prior to a yield point, but that egress of these dislocations is inhibited by the oxide film. Upon fracture of the oxide film, this constraint is lifted and elastic/plastic indentation ensues.

11:00 AM W6.8/8.8

EFFECT OF SURFACE STEPS ON DISLOCATION STRUCTURE DURING NANOINDENTATION. Jonathan A. Zimmerman, Patrick A. Klein, Stephen M. Stiles, Stanford National Labs, Livermore, CA.

The study of dislocation nucleation and plastic behavior during nanoindentation is a prime example in which nanoscale details play an important role in the evolution of macroscale mechanical behavior. Experimental studies of nanoindentation suggest that the presence of surface irregularities, such as steps, modify the mechanical response during indentation. However, the experiments did not reveal the details of dislocation creation or how the nucleation process is altered by the irregularities. Through quasistatic and dynamic simulations using the embedded atom method, we examine the indentation of an Au(111) crystal that contains a surface step. These simulations show the effect of the presence of the step on both global quantities of indentation force and mean pressure as well as the local atomic stresses. A new formalism for atomistic deformed structure, the slip vector, is used to quantify initial dislocation content. Using this metric, we analyze the shear stresses resolved onto the directions of the partial dislocations that form, improving upon previous analyses which have used the maximum resolved shear stress of all possible slip directions. Our analysis leads to an estimate of critical resolved shear stress to be understood in terms of a nucleation criterion even at very low distances to atomic level defects, such as a surface step. In addition, the dislocation stress fields are compared with continuum calculations performed using an elastic, Casady-Born elasticity. These results show that the dislocation fields correctly reproduce the large deformations close to the indenter. The use of this model in conjunction with a coupled atomistic-continuum approach would allow simulation of systems much closer in size to those studied in experiments.

11:15 AM W6.9/8.0

IDENTIFICATION OF PRESSURE-INDUCED PHASE TRANSFORMATIONS USING NANOINDENTATION. Vladislav Domnich, Univ of Illinois - Chicago, Dept of Mechanical Engineering, Chicago, IL; Vary Gogotsi, Drexel Univ, Dept of Materials Engineering, Philadelphia, PA.

Depth-sensing indentation has been successfully used for identification of pressure-induced phase transformations in several brittle materials. Phase transformations during indentation may be revealed though changes in the load-displacement curve, called "pop-in" or "pop-out" events. Skaggishlock transformation is followed by a gradual change in the slope of the loading or unloading curve (in elbow), which may not always be readily identified if the indentation data are presented as the load-displacement curves. Based on the empirical power law relation between the applied load and the elastic part of the indenter displacement, the average contact pressure [Meyer's hardness] during indentation can be assessed as a function of the contact depth between the indenter and the specimen. This technique has been applied to cupolas and other soft materials, such as silicon, germanium, boron carbide and zirconia.

11:30 AM W6.10/8.10

MECHANICAL DEFORMATION OF CRYSTALLINE SILICON DURING NANOINDENTATION. Jodie Bradley, J.S. Williams and J. Weng-Liang, Australian National University, Department of Electrical and Electronic Materials Engineering, RSIP Tech, Chatswood, NSW, AUSTRALIA; M.V. Swain, University of Sydney, Biomaterials Science Research Unit, Department of Mechanical and Mechatronics Engineering and Faculty of Dentistry, Sydney, NSW, AUSTRALIA; P. Morse, University of New South Wales, Electron Microscope Unit, Sydney, NSW, AUSTRALIA.

Deformation during spherical and pointed indentation in (100) crystalline silicon using a UBM-S200 nanoindentor has been studied using cross-sectional transmission electron microscopy (XTEM). Atomic force microscopy and Raman microspectroscopy. XTEM samples were prepared by focused ion beam milling to accurately position the cross-section through the indentation. Indentation loads were chosen below and above the yield point for silicon to investigate the effects of plastic deformation. Slip planes (originating from the region of maximum shear stress) are visible in XTEM micrographs for all indentation loads studied but slip is not the main route for plastic deformation. A thin layer of polycrystalline material has been identified (indexed as a high pressure phase from diffraction patterns) on the low load indentation, just prior to yield (pop-in during loading). For loading above the yield point, a large region of amorphous silicon was observed directly under the indenter when fast unloading conditions were used. The various microstructures and phases observed below indentations are correlated with load/unload data.

11:45 AM W6.11/8.11

AN ASSESSMENT OF THE MICROSTRUCTURES AND MECHANICAL STRENGTHS OF ALUMINIDE-BASED THIN COATINGS. S.Y. Li, H.P. Ng and Alfonso H.W. Ngan, Univ of Hong Kong, Dept of Mechanical Engineering, Hong Kong, PR. CHINA.

Titanium and nickel aluminide-based thin coatings were synthesized by magnetron sputtering from intermetallic Ti50at.%Al and Ni-25at.%Al alloy targets on various substrate materials. Both of the aluminide coatings exhibited a surface hardened structure compared to the substrates, while the Ni-alloy coating was similar to the substrates, while the Ni-alloy coating was similar to the substrates. The analysis indicated that the strengths of the aluminide coatings considerably exceed their strengths in bulk. Plasibased strengthening mechanisms are discussed.