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 STIFFNESS AND LIMITS OF STRENGTH IN THEORY AND ATOMIC SIMULATIONS
Ji 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 homogenous material in terms of bond-dependent elastic stiffness coefficients. These criteria provide upper bounds on the material's strength, approachable sometimes in indentation hardness experiments. The extension of homogenous deformation to finite wavelength is the analysis of phonon soft mode for a stressed lattice is inhomogeneous at finite temperature. We will present lattice dynamical results obtained using model potentials for a variety of solids [Ar, Cu, Mo, Si, SiC, SiO₂, 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 heteropolynuclear 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 at the available timescales, lattice re-arrangements are too little 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 SiO₂ UNDER EXTREME CONDITIONS OF PRESSURE AND TEMPERATURE. M.J. Caturia, A. Kubota, T. Lenkosky, V. Buhtov, T. Do 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 atom-scale mechanism of crack growth in silicon under extreme conditions of pressure and temperature. In this presentation we will describe our parallel molecular dynamics code MDCASK by including multidimensional expansion algorithms to describe long-range covalent interactions. We compare several empirical interatomic potentials with ab initio (GGA) calculations under different tensile-strain fields in order to select that empirical potential that is most suitable for this study. We show interesting trends in SiO₂ fracture properties of pre-existing cracks as a function of varying 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 favorable 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 plane. The calculation suggests that the crack plane is the plane of highest anisotropy, as expected from the energetics of the crack tip.

84 crack tip bonds smoothly with increasing load and cracks propagate easily on (111) and (110) planes provided crack propagation processes in the (110) direction. This continuous process mimics what we would expect from continuum theory and therefore results only in a small lattice trapping. In contrast, if the crack is driven in a (001) direction the crack front propagation 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 behaviour can be partly traced back to some bond breaking of the crack tip bond and the neighboring bonds, which effectively shields the crack tip bond from the applied load and results in a large lattice trapping region. Different lattice trapping for different crack propagation directions can explain the experiments observed cleavage anisotropy in silicon single crystals.

9:30 AM W1.4
INFLUENCE OF CRYSTALLOGRAPHIC SYMMETRY ON ELASTIC STIFFNESS AND BIFURCATION PHENOMENA AT FINITE STRAIN. Frederick Miloteln, 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 post-bifurcation phenomena leading to phase change or material failure, as predicted by elastic stability theory. The mechanical response, including theoretical predictions, is strongly influenced by crystal symmetry and associated bifurcation behaviour. Prominent 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 of (c11, c12, and c44) and the three sixth order moduli of (c111, c112, c123, c144, c166, and c444) of 12 cubic metals [Al, Cu, Mo, Na, Li, K, Rh, Nb, Fe, Ni, Au, and Ag]. This formulation ensures that the transition between linear and non-linear (anharmonic) response of the metals is represented in the computations. Examples of both lattice static and molecular-dynamic results are presented.

10:30 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 DEFORMATION IN METALS. Nicholas Kizaka, M. Hermanson and E. Collins, 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 plane 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 are perpendicular to the bond path variably in the unstable stacking fault configuration.

Supported by U.S. Army Research Office.

11:15 AM W1.7
THEORETICAL TENSILE STRENGTH IN METALS AND INTERMETALLICS. M. Sch, L. G. Wang, M. Friček, Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Prague, CZECH REPUBLIC; V. Vitek, 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 elastic anisotropy of the higher strain are closely connected with the presence or absence of higher-symmetry structures along corresponding deformation paths. Tensile 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-dictated energy extrema corresponding to cubic lattices depending on the atomic ordering. However, other energy extrema 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, NiAl and MoSi2 loaded uniaxially along principal crystallographic directions will be discussed.


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 (S) 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 F49620-96-1-0246.

SESSION W2
Chair: Peter Gumbsch
Tuesday Afternoon, November 28, 2000
Fairfax B (Siersson)
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 microscopic and macroscopic 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 plastic data on bcc metals [1] and semiconductors [2, 3] have been consolidated into universal relations describing the temperature dependence of the flow stress. 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 (Pt-Pu) or boron nitride (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 flowstress 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. L. Shi, University of Iowa, Dept of Civil and Environmental Engineering, Iowa City, IA, Jimmei Huang, Nurn M. Gloniem, 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, protons or laser light, and in metals quenched from high temperatures or subjected to high-shear rate 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 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 mechanism of dislocation interaction with interstitial defect clusters are also analyzed by DD; it is found 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, and as mixed discrete-continuum computations of the Peierls-Nabarro type for fcc metals. One of the reasons for this is that for 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, there are the first atomistic computations of the Peierls stress of edge or mixed dislocations for an fcc metal.

2:45 PM W2.5 ATOMIC VIEW OF THEORETICAL STRENGTH OF BCC METALS: CORE STRUCTURE AND MOBILITY OF 1/2<111> SCREW DISLOCATION IN Ta. Guangfeng Wang, Alejandro Strachan, Tahir Cagin, William A. Goddard, III, California Institute of Technology, Materials and Process Simulation Center, Pasadena, CA.

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 1/2a<111> screw dislocation. Equilibrated core structures were obtained by relaxation of dislocation quadrupoles with periodic boundary conditions. We found that the equilibrium dislocation core has three-fold symmetry and spreads out into three <112> directions ([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, with <112> or <110> dipole orientation. In both cases the dislocations move in zig-zag 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 μ, where μ is the bulk shear modulus of perfect crystal. The preferred slipping direction is in [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 which 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 BRITTLE FRACTURE OF IRON BY ULTRA GRAIN REFINING: Kotobu Naka, National Research Institute for Metals, Bunkyo, JAPAN.

Low temperature brittleness is thought as an inevitable phenomenon for low-carbon steels like Ni-Cr steel. 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 samples containing the ultrafine grains large enough to take full-size impact test pieces for a low carbon steel. The DBTT of such ultrafine grain steels was found to be 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 pearlite 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 limitations of strength in tension suggest that bcc metals necessarily cease on (110) at a tensile stress of about 0.08E(110) while for fcc metals cease if (111) at a tensile stress of 0.12E(111). For deformation analyses of the normal stress in the stress concentration region ahead of a sharp 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 limit’ is exceeded by a number of existing alloy steels, but is not approached in structural aluminum alloys.

4:15 P.M. W2.8
ULTRAFINE GRAIN REFINEMENT BY HEAVY DEFORMATION OF SUPERCOOLED AUSTENITE AT JUST ABOVE Ar3. Chang Sun Lee, Jae Sung Lee, Jong Kyo Choi, Won Yong Choo, POSCO, Pohang, R&D & Welding Research Team, Pohang, KOREA.

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 curves during deformation, dislocation density after deformation, 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 analysis of dislocation density curve 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 and amount of deformation and austenite 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. V. Yamakawa, D. Wolf, S.R. Phillpot, and A. Gali, National Laboratory, Argonne, IL; H. Gleiter, Forschungszentrum Karlsruhe, Karlsruhe, GERMANY.

Molecular-dynamics simulations are used to elucidate the low-temperature, tensile-deformation behavior of nanocrystalline fcc 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, initially 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-dominated deformation process. 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. Responsible for flow behavior is a process of grain refinement 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 a highly elongated grain. 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-31109-Eng-38.

4:45 P.M. W2.10
PHASE FIELD MICROELASTICITY APPROACH TO DYNAMICS OF DISLOCATION SYSTEM. Yu U. Wang, Rutgers Univ., Dept. of Mechanical and Aerospace Engineering, Piscataway, NJ; Yongmei M. Jin, Rutgers Univ., Dept. of Ceramics and Materials Engineering, Piscataway, NJ; Alberto N. Garan, Rutgers Univ., 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 well as full-field finite element solution, does not impose any prior constraints on dislocation patterns formed during the evolution. The Phase Field Dislocation model is used to simulate the mechanical behavior of materials 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: Nasr M. Ghoniem
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 FRAC TURE 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 both by 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 or research focus is warranted.

9:00 AM W3.2
DISCRÈTÉ DISLOCATI ON SIMULATION OF THIN FILM PLASTICITY INCLUDING TAILLORG, Argonne, IL; H. Gleiter, Forschungszentrum Karlsruhe, Karlsruhe, 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. 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 is also shown that the optimum orientation distribution 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 Hill-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.

9:15 AM W3.3

Quantitative experimental observations of dislocation nucleation and glide in the model Al (001) / 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 (001) 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 in situ transmission electron microscopy allows real time observation of dislocation climb, cross-slip, grain boundary nucleation and glide. In this work, it was found that dislocation nucleation occurs preferentially at the c-axis in the grain boundaries, beginning at a temperature of 275°C, followed by slip along the inclined (111) glide planes. Subsequent microstrain measurements of 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. Quantitative observations on all four n<2 c<<0 {111} slip planes. Hence, we show that the observed plastic behavior is a direct result of the anisotropy of stress in the (001) 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 that in the perpendicular (111). 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 TAILLEFILM METALLIC THIN FILMS. Massimo J. Kolobovsky, Carl V. Thompson, MIT, Dept. of MSE, Cambridge, MA; Mihal E. Gross, Bell Labs, Lucent Technologies, Murray Hill, NJ.

While the fine microstructure of polycrystalline metal 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, we perform inelastic deformation measurements on submicron-sized 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: dislocation creep and dislocation-mediated plasticity controlled by the thermally activated motion of dislocations through obstacles, which presumably are forest dislocations. As expected, dislocation creep is dominant in 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 disfacial 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 dominates and controls 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 for all grains with decreasing thickness and grain size. This behavior is the result of the interplay between dislocation-mediated plasticity and dislocation-mediated creep.

10:15 AM W3.5
STRESS DEPENDENT STRUCTURE OF 90° PARTIAL DISLOCATION IN Si. Lin, D.C. Chao, Department of Physics, University of California, Berkeley, CA and Center for Advanced Materials; Ernest Orlando Lawrence Berkeley National Laboratory, Berkeley, CA. 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 conducted using a full atomistic 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 stress and 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.

10:30 AM W3.6
ATOMIC SIMULATION OF KINK-PAIR ENERGY IN SCREW DISLOCATIONS IN BCC 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, National Institute of 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, or vice versa. In this work, the nudged elastic band method is used to calculate the activation path connecting such jumps. Kink-pairs are found to involve in all such jumps. These kink-pairs are denoted according to the Devonshire scheme as "BaAp", "AnBa", "AnA" and so on, where n and p denote the signs of the kinks, the first and third and 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 heterohomorphous kink-pairs, BaApB and AnBaB, and one homophomous kink-pair, AnBaApA. The simulation results also show that the energy of these kink-pair BaApB has significant Born-Huang activation energy than the other heterohomorphous kink-pair AnBaB as well as the homophomous kink-pair AnBaApA. 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 when a "positive" applied stress is applied. The difficult jump on the primary [101] plane can however be bypassed by jumping onto an intersecting cross-slip plane, the morphological which is equivalent to the easy jump on the primary plane. The motion of the screw core would therefore be zigzagging and the average slip plane would tend towards the msa plane. We believe this is the proper explanation of the observed pencil glide at elevated temperatures. The activation energy of the screw-dislocation BaApB kink-pair is thermally activated by more than 0.5 eV, which means the limiting strength process, 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 from layer to layer. In this regime, the strength monotonically increases with decreasing layer thickness. At smaller layer thickness, the strain 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 Pb stimulated interest in this apparent inverse Hall-Petch behavior for decreasing grain size in the nanocrystalline regime. However, it was subsequently pointed out that for most of the experiments where inverse Hall-Petch behavior was observed, the grain size was obtained by reducing 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 these 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 for 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 intrinsic dependence of the stress-strength and strain with grain size are 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.

11:15 AM W3.8
THE TEMPERATURE DEPENDENCE OF MICROCRACK ARREST IN FERRITE AND ITS RELATIONSHIP TO A UNIVERSAL MASTER TOUGHNESS CURVE SHAPE. M. Holmenk, G.R. Odette, and M.V. Re, University of California, Santa Barbara, Dept of Mechanical and Environmental Engineering, Santa Barbara, CA.

Considerable empirical evidence suggests that the climb initiation toughness curve for structural steels in the brittle to ductile transition has an approximately universal Kc=(T-Tf)/Tf on a relative temperature scale (T-Tf) but have relatively little impact on the master curve (MC)-type shape. A new micromechanical model combining analytical representations of low element analysis (FEA) simulations of crack tip stress fields with a local critical stress-critical area (σ*c, A*) fracture criterion is consistent with a universal MC shape if the σ*c increases monotonically with temperature where the yield stress approaches its normal limit. The σ*c is the stress necessary to propagate a dynamic microcrack from a broken trigger particle, and is usually given by a Griffith-type criterion related to the size of the trigger particle and the microscale toughness of the material, Kmirc. Thus, the most general and fundamental explanation of a universal MC shape, is a corresponding increase in Kmirc with temperature. Various experimental approaches to evaluating Kmirc[T] are described, including measurement of crack arrest toughness in oriented iron single crystals. This method involves compression to a known compressive deformation followed specimens composed of a brittle phase region to dynamic crack initiation and an oriented single crystal crack arrest region embedded in polycrystalline iron compression loading bar. The implications of the observed Kmirc[T] behavior to the shape of the MC are described along with a dislocation dynamics model.

11:30 AM W3.9
LOCAL AND GLOBAL FAILURE MODES IN POLYCRYSTALLINE AGGREGATES. W.M. Ashawi and M.A. Zikry, North Carolina State University, Department of Mechanical and Aerospace Engineering, Raleigh, NC.

A multiple-slip dislocation-density based constitutive formulation and specialized computational schemes have been developed to characterize material failure on the appropriate physical scales needed for the current understanding of physical mechanisms that control failure initiation, growth, and coalescence. Dislocation-density transportation and blocking interfacial conditions and local stress fields have been obtained for grain-boundary distributions associated with random and tilt orientations. These evolving local stress fields are used as failure criterion to track the initiation and evolution of intergranular and transgranular fracture. The interrelated effects of grain boundary orientation, dislocation density pile-ups and evolution, geometrical and thermal load and parallel to interfaces. A consequence is that the hydrostatic stresses on failure paths in cubic crystalline materials have been studied. Based on the present analysis and on comparison with experimental observations, it is shown transgranular and intergranular failure can be characterized in terms of the competition between the strengthening and the softening mechanisms of the crystalline structure.

SESSION W4/1B5 JOINT SESSION
Chair: Deryl C. Chrien and Richard G. Hwang
Wednesday Afternoon, November 29, 2000
Room 310 (Hynes)

1:30 PM W4/1B5.1
THE INVERSE HALL-PETCH EFFECT - FACT OR ARTIFACT. Carl Koch, North Carolina State Univ., Dept. of MSE, Raleigh, NC.

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 size, strain rate, and temperature, have been studied using quasi-static and high strain rate (Kolsky bar) tests. Ultrafine grain sizes, Fe exhibits high strength, little work hardening, and plastic straining 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 5E5/s). 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 grain sizes and strain rate, temperature, the yield strength decreases and plastic strain increases. These findings are compared with the Hall-Petch relationship, and examined to derive the validity range, in terms of grain size, temperature, strain rate, and particle bonding strength, of different deformation mechanisms (e.g., dislocation mechanisms). In addition, we comment on the potential advantage of related alloys for military kinetic energy penetrators where the shear banding mode and shock-hardenability capability during high rate deformation is desired.
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 (of typically 10^5 s), our input microstructures were tailored to (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 simulations showed that the steady-state diffusion creep is governed by a diffusion process (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 understanding of the fast creep effect, is discussed.

value $V$ 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&IE, University of Illinois, Urbana, IL.

Thermally-activated plastic deformation in single crystal silicon is studied. Samples oriented for single slip are loaded by a dead-weight in an isotherm, the shear strain rate is measured using 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 between stress and the critical temperature is used to determine 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. F. Rochedi 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 (i.e. tensile stress) by the reflection of a 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 presented here: this explanation suggests a hitherto unsuspected mechanism for the control of magnitude discrepancies in dynamic tension tests on previous dynamic stressing experiments. We present a new method of estimating the effective tensile strength of liquids using an extrapolation procedure in the range of static positive pressures. This method, which provides estimates 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 deionized water can sustain a tensile tension of nearly 350 bar, recharging 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 multi-grade motor lubricants at elevated temperatures.

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

Mechanical, geometric, and kinetic characteristics of crystal instabilities are revealed via microscopic 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 Milstein. Fluctuation models are used for computation of elastic moduli employed in measurements of elastic stability. Interatomic interactions in metals are expressed both by simple Morse pair potentials and by more accurate semi-empirical embedded-atom methods. Results have been parameterized specifically for studies of crystal elasticity at finite strain. As an example, the stability of hcp crystals was studied under constant pressure and temperature. It was found that the evolution of elastic stability criteria predict the onset of hcp-to-hcp transitions. Computations were carried out of the crystals' shear moduli in each pressure and temperature condition of the evolution of the crystals' enthalpies along the transformation path. Under anharmonic conditions, the hcp-to-hcp transitions proceeded according to the Burgers mechanism. Most importantly, the transitions were constrained by the presence of a pressure pulse at a crystal's strain rate. The critical shear strains 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.

Mizumori Kobayama, Dept of Mechanical 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 methodology based on 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 and with S-N-1 boundary are examined. 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 tests, the supercell is in a small increment, and all the atoms are relaxed. This cycle is iterated until the interfaces are broken. The corresponding to a real tensile test at 300 K. Young's module, tensile strength, fracture energy, and fracture toughness are obtained for these interfaces. Features of fracture, bond breaking and changes in the electronic structure are analyzed 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 wrong 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 (> 8 GPa) a-D films, since thermal annealing to moderate temperatures (300°C) can completely remove the stress without significantly changing the 4-folds 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 tests structures) to evaluate the micromechanical properties of these films. For example, early tensile test results done without an indentor show that the a-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 350°C. Furan analysis of the annealed a-D films shows that the character of the 3-fold carbon bond change with annealing while EELS on plan-view samples indicates almost no change in the 4-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 topology and attempt to confirm the 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. Ferenczak Elezhani, MSE&IE Dept., University of Florida, Gainesville, FL.

We have fabricated nanocrystalline 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, microhardness analysis, 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 concentration of impurities or intergranular boundaries. Excessive cooling of hydrogen resulted in formation of ultra-fine voids, which led to microvoid coalescence fracture mechanism. Otherwise, all electrodeposited single-phase FCC nanocrystals fractured 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 lamination nanostructures consisting of two different metallic layers with FCC crystalline structures, however, showed cleavage-like facets. One explanation is that local stress is high as the theoretical strength develops in nanocomposites materials. The other possibility is that deformation at interfaces or a high density of processing voids provide the opportunity for testing of ultra-fine ligaments, which look like cleavage facets. The possibilities of these mechanisms are discussed in Cu/Ag and Cu/Ni nanocrystallized structures.
thin films studied by microbeam x-ray diffraction (μXRD) 

Plasticity in thin films has been extensively studied by macroscopic mechanical techniques such as uni and tensile testing, but is still partially understood. In the present work, we have investigated the plastic phenomena by using Microbeam X-ray Diffraction (μXRD) combining monochromatic x-ray beam and detectors.

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 techniques of CBED (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 patterned Cu blanket films (0.3 - 1.5μm thick) was studied between room temperature and 300°C. Furthermore we measured effects of two-dimensional confinement of passivated Al lines (0.7μm wide) and passivated and unpassivated electroplated Cu damascene lines (0.8 - 5μm wide) at temperature varying from room temperature to 300°C.

The results indicate noticeable changes in strain and texture variations within individual single grains.

W5.12 DETERMINATION OF STRESS ORIENTATION DISTRIBUTION FUNCTION IN POLYCRYSTALLINE MATERIALS WITH NEUTRON DIFFRACTION, Yeongdoo Wang and Yun-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 large anisotropy of elastic or plastic behaviours 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 mean-field 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, 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/Au3O3 INTERFACE, S.S. Mac, Department of Mechanical Engineering, University of Pittsburgh, Pittsburgh, PA.

Interfacial strength and fracture at Au/Au3O3 interface in layered materials are investigated for Au layered on Au3O3. Fracture testing has been carried out to measure the interfacial strength and toughness using Au3O3/Au3O3 sample. The associated interfacial strength of Au/Au3O3 in 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 layers is considered, and the energy for initial emission of a dislocation is assumed to be obtained before the cleavage of the interface crack. Superdislocation modeling is employed to obtain the critical strain energy release rate, for interface separation from crack tip. When a stress separation has been initiated by a dislocation, an 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/Q8: JOINT SESSION
LIMITS OF STRENGTH IN INDENTATION
Chairs: Murray S. Daw and Jost J. Višnec
Thursday Morning, November 30, 2010
Room 309 (Hynes)

8:30 AM W6.1/Q8.1
EXPERIMENTS ON THEORETICAL STRENGTH AND SIZE EFFECTS IN JOURNAL INDENTATION V. D. Nix, Rajrajan Suha, Eric T. Lillicoeid, 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 multi-scale 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 Ta 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 the grain boundaries can play a role in dislocation nucleation. Here 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 gradient plasticity. 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 metal 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 failing hardness with increasing depth in bulk materials. We associate this rise in hardness with the strong gradient of plastic strain created between the indenter and the substrate. We show that it is calculated using a recently developed model of strain gradient plasticity.

9:00 AM W6.2/Q8.2
CONNECTING ATOMIC AND EXPERIMENTAL ESTIMATES OF IDEAL STRENGTH. C.R. Krenn1,2, D. Roundy2,3, Marvin L. Cohen2,3, D.C. Chrzan1,3 and J.W. Morris Jr.1,3. 1Univ. of California at Berkeley, Dept. of Materials Science and Chemical Engineering, 2Univ. of California at Berkeley, Dept. of Physics, 3Lawrence 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. Using non-indentation techniques, it is also possible to experimentally apply stresses of the order of the ideal shear strength to defect free regions of high purity single crystal. However, realistic determination of the stress fields produced during high strain non-indentation requires finite element modeling. We use a finite element model incorporating a nonlinear stress-strain curve of the form that is calculated ab initio for boron to determine the maximum shear stresses reached beneath a spherical indenter on a nonlinear elastic substrate. This model yields a load-displacement curve very similar to a Hertzian nonlinear elastic solution, but the peak shear stresses beneath the indenter are only 70% of those obtained from the Hertzian solution. We use these results to compare ab initio ideal strengths with the maximum shear stresses reached during nanoindentation 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 nanoindentation is not reached initially, but is reached only under the initial load-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/Q8.3
THE ROLE OF MICROSTRUCTURAL LENGTH SCALE IN DEFORMATION BEHAVIOR OF GOLD. Erica T. Lillicoeid, William D. Nix, Stanford University, Dept. of MSE, Stanford, CA.

Observations of depth dependent hardness have been made for various materials, 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, imparting 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 dislocation distributions and strength. It is shown 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 in 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/Q8.4
PHYSICAL ORIGIN OF A SIZE EFFECT IN NANO-INDENTATION. A.J. Bushby1, J.R. Downes2, N.B. Jayaweera2, P. Kidd2, A. Kelly3 and D.J. Thostenson3. 1Department of Materials, 2Department of Physics, Queen Mary and Westfield College, University of London, UNITED KINGDOM, 3Dept. of Math & 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 high and low Young's modulus. The yield pressure is reduced by the presence of the coherency strain. By varying the thickness and strains, we have been able to show that both sets of layers, compressive and tensile, reduce the yield pressure. This implies that a yield criterion must be satisfied over a finite volume, large enough to include layers of both sign. In these studies, we have observed a large and reproducible size effect in the yield pressure. That is, with smaller radius indenters the mean pressure acting over the contact area at the deviation from purely elastic behaviour increases, by up to a factor of two, from a 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 found. This is in contrast to the understanding of nanoindentation and other systems in which stresses are highly heterogeneous on a small scale.

9:45 AM W6.5/Q8.5
IN-SITU NANOINDENTATION 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. Stud, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA; C.R. Krenn, J.W. Morris, Jr., Department of MSE, University of California, Berkeley, CA and Center for Advanced Materials, Lawrence Berkeley National Laboratory, Berkeley, CA.

The mechanics of nonmechanical deformation in ultrathin materials such as the transition metal carbonitrides are poorly understood. We have recently developed a nanoindentation TEM specimen holder which gives us the ability to make real-time observations into the nonmechanical response of various materials. We will show results from real-time nanoindentations of transition metal carbonitrides and the subsequent analysis of the resulting indentation damage. Our results will be compared to prior ex-situ indentation of ultrathin 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.

10:30 AM W6.6/Q8.6
MECHANICAL RESPONSE OF DIAMOND AT NANO-METER SCALES: DIAMOND POLISHING AND AFM. Ruben Pérez, Murray R. Jarvis and Michael C. Payne, Universidad Autonómica de Madrid, Departamento de Fisica Teorica de la Materia Condensada, Madrid, SPAIN; University of Cambridge, Theory of Condensed Matter, Cavendish Laboratory, Cambridge, UNITED KINGDOM.

Many technological processes and characterization techniques rely on the mechanical response of materials at the nanometer scale. Although computationally demanding, ab initio methods can now be used to explore the limits of strength with strain under a variety of conditions. In this work, total energy pseudopotential methods are used to study two different processes involving the mechanical interaction of diamond
nanoparticles and diamond surfaces: the wear processes responsible for diamond polishing, and the mechanical deformation of tip and surface during nanoindentation of the Nanoindentation Mechanism (CM-AFM). The strong symmetry in the rate of polishing between different directions on the diamond [110] surface is explained in terms of an anisotropic mechanism for nano-geometry wear. Although anisotropic behavior is not inherent to the diamond, the direct observation of material transfer during polishing is still of interest. The wear process can be studied in two steps. Separate simulations in which a rigid tip was incident on the soft and the hard polishing directions on a single nano-scraper show pronounced differences in the indentation process. The difference in the normal indentation force with respect to the direction of the nano-crystalline and non-crystalline material. A sudden volume change during the indentation process is caused by the indentation in the load-displacement curve ("pop-in" or "pop-out" events). Such indentation is followed by a gradual change in the slope of the unloading or unloading (curves), which may not always be readily identified if the indentation data are presented as the load-displacement curve. 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. Defined in this manner, the pressure - depth relation is linear unless the elastic modulus of the specimen changes in the process of indentation. This greatly facilitates monitoring of possible phase transformations under the indenter and silica assessing the corresponding transformation pressure. Phase changes after indentation are verified by Raman microspectroscopy. The technique is applied to the studies of several single crystal semiconductors and ceramics, including silicon, germanium, boron carbide and zirconia.

11:30 AM W6.10/08.10 MECHANICAL DEFORMATION OF CRYSTALLINE SILICON DURING NANOINDENTATION: Jodie Bradley, J. William and J. Wendt, Boston University, USA. Nanocrystalline diamond (c-ND) and silicon micro/nanoindentation. The samples were prepared by focused ion beam milling to accurately position the cross-section through the indentations. Indentation loads were chosen below and above the yield point for silicon to investigate the modulus of plastic deformation. Slip planes (originating from the region of maximum shear stress) are visible in TEM micrographs for all indentation loads studied but slip is not the main avenue for plastic deformation. A thin layer of poly-crystalline 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 W6.11/08.11 AN ASSESSMENT OF THE MICROSTRUCTURES AND MECHANICAL STRENGTHS OF ALUMINIDE-BASED THIN COATINGS: S.Y. Li, H.P. Ng, and Alfonso H.W. Ngan, University 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 Ti5Al5Ni and Al2Ni, 50 nm targets on various substrate materials. Both of the coatings exhibited a surface hardness of 35.0 GPa, with the coating formed with the degree of heat treatment. Structural characterization using atomic force microscopy and transmission electron microscopy revealed a typical nanocrystalline structure in the coatings. The hardnesses of the coatings were investigated over a wide range of applied stresses using micro- and nano-indentation techniques. It was found that the measured hardness of the coatings depends on the indentation depth, the film thickness as well as the strength of the substrate. In order to estimate the stress-strain behavior of the films, the indentation size effects of the apparent hardness were analyzed in terms of the "absolute hardness" models by Johnson and Hogmark (1981) and Ngan and Ng (submitted). The Johnson-Hogmark model is more applicable to the situations on the different substrate materials, while the other model is applicable to soft films on either soft or hard substrates. The analysis indicated that the strengths of the aluminode coatings considerably exceed their strengths in bulk. Plausible strengthening mechanisms are discussed.