SYMPOSIUM Z

Multiscale Materials Modeling

November 27 – December 1, 2000

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* Invited paper

8:30 AM *Z1.1
ISSUES IN THE TRANSITION FROM DISCRETE DISLOCATION
TO STRAIN GRADIENT CONTINUUM PLASTICITY.
Erik Van der Giessen, Delft Univ of Technology, Koiter Institute,
Delft, THE NETHERLANDS; Alan Needleman, Brown Univ, Division
of Engineering, Providence, RI.

Continuum theories of plastic flow attempt to average out over the
slips created by many dislocations. Detailed information about the
individual dislocations and their interactions is lost during the
averaging process, and only the overall effect enters the continuum
description through a plastic flow rule. There is a significant literature
on relating continuum-level plastic flow properties to discrete
dislocation processes. For example, the effect of forest dislocations
and other obstacles on the flow strength and hardening of crystalline
solids has received a great deal of attention from various researchers
and considerable progress has been made. An issue that has received
much less attention is related to the fact that a discrete dislocation
description of plastic deformation is intrinsically non-local. Since a
formal and workable averaging scheme over many discrete dislocations
has yet to be developed, the form a nonlocal continuum plasticity
theory should take remains to be established. Various theories have
been proposed having very different mathematical structures. One
means of differentiating between these competing formulations is by
comparing their predictions with corresponding predictions obtained
directly from discrete dislocation plasticity. Here, some recent
comparisons made for two-dimensional model problems are
summarized. These include a composite with elastic inforcements and
a single crystal between two passivation layers. Discrete dislocation
results for single and double slip are compared with the predictions of
various nonlocal continuum plasticity theories including those of
Acharya and Bassani and of Fleck and Hutchinson.

9:00 AM Z1.2
MULTISCALE MODELING OF DISLOCATION PROCESS IN BCC
TANTALUM: BRIDGING ATOMISTIC AND MESOSCALE
SIMULATIONS. Lin H. Yang, Meijie Tang, and John A. Moriarty,
Physics Directorate, Lawrence Livermore National Laboratory
Livermore, CA.

Plastic deformation in bcc metals at the low-temperature and
high-strain-rate is controlled by the motion of a/2<111> screw
dislocations. Understanding the fundamental process of screw
dislocation motion in bcc Ta is the focus of our present study. The
multiscale modeling approach presented here is based on information
passing, where results of simulations at the atomistic scale are used in
simulations of plastic deformation at micron length scales via
dislocation dynamics[1]. The intrinsic core properties of a/2<111>
screw dislocations have been simulated by means of volume-dependent
multi-ion interatomic potentials, which are derived from model
generalized pseudopotential theory (MGPT) and an accurate ab-initio
data base, and the flexible boundary conditions [2]. The
stress-dependent results on the fundamental kink-pair mechanism and
orientation-dependent Peierls stress were then used as input for
dislocation dynamics simulations. The later is based on a screw-edge
model in a discretized lattice where the dislocation mobilities are
critical input to the study of non-Schmid effect. Results will be
analyzed in comparison with experimental data.
[1] M. Tang, L.P. Kubin, and G.R. Canova, Acta Mater. 46, 3221
(1998).
[2] L.H. Yang and J.A. Moriarty, Mater. Sci. and Eng. A, in press; L.
H. Yang, Per Sderlind, and J.A. Moriarty, to be published.
*This work was performed under the auspices of the U.S. Department
of Energy by the University of California Lawrence Livermore
National Laboratory under contract number W-7405-ENG-48.

9:15 AM Z1.3
SIMULATION OF MULTI-SLIP DEFORMATION OF Mo USING
DISLOCATION DYNAMICS. M. Rhee, V. Bulatov, L. Hsuing, D.
Lassila and T. Diaz de la Rubia.

New efficient version of LLNL's micro3d code incorporates several new
developments in the Dislocation Dynamics methodology. These
include a general mobility rule based on the atomistic results for
kink-pair mechanisms of dislocation motion and a full 3D
implementation of the periodic boundary conditions. The latter
technique is an efficient way to simulate crystal plasticity in the
material bulk in which the dislocation flux balance across the
simulation volume is naturally preserved. The resulting method is free
of various artificial effects associated with all other types of boundary
conditions currently employed and is well suited for treating very
large collections of interacting dislocations. Based on this new

approach, a large-scale Dislocation Dynamics simulation of plastic
deformation in single crystalline Mo reveals interesting details of
micro-yield and strain hardening behavior.
This work is performed under the auspices of U.S. Department of
Energy and Lawrence Livermore National Laboratory under contract
No. W-7405-Eng-48.

9:30 AM Z1.4
INTERACTION OF DISLOCATIONS WITH A FREE SURFACE.
Xiao Hu Liu and Klaus Schwarz, IBM Research, Yorktown Heights,
NY.

Image forces arising from the presence of free surfaces or interfaces are
often very difficult to calculate. Although such forces are generally
very important for 2D problems and other situations involving
straight dislocation lines, the matter is less clear for curved
dislocations, where the self-interaction often plays a dominant role. In
many situations, it may even be sensible to neglect the image
corrections to first order. To explore this issue, and to test various
approximation schemes, we have performed accurate calculations of
the behavior of dislocations which pass close to or which actually
terminate on a free surface. To do this, each such dislocation is
surrounded by a highly resolved surface grid, the tractions on this
grid then being used to compute the stress tensor and to move the
dislocation by utilizing the well-known Boussinesq-Cerruti formalism.
The singular region where a dislocation touches the interface is
treated by a line-splitting procedure consistent with that used to treat
the self-interaction. Results will be presented which support the view
that for many problems of current interest, the neglect of image forces
does not introduce errors much greater than the 10-20% range already
inherent in continuum dislocation dynamics.

9:45 AM Z1.5
3D DISLOCATION DYNAMICS IN BCC METALS WITH THE
PARANOID CODE. L.K. Wickham, Lawrence Livermore National
Lab, Livermore, CA; K.W. Schwarz, IBM T.J. Watson Research
Center, Yorktown Heights, NY.

We present results of large−scale simulations of three−dimensional
dislocation interactions in bcc metals using the PARANOID
(PARAllel NOdal IBM Dislocation) code. We show tangles which
develop from collections of initially straight dislocations at various
densities, mobility anisotropies, and external stresses. We also give
the results of simulations whose dislocations start with a finite density
of large jogs. Such jogs have been observed in annealed samples of bcc
metals and have been of key interest in recent simulation work at
L.L.N.L.. We find that, even when these jogs are allowed to relax and
elongate, they can gather up under external stress and produce loops
which resemble those observed in strained TEM specimens. We also
plan to discuss effects of different boundary conditions.

10:30 AM *Z1.6
ON GRADIENT DISLOCATION DYNAMICS. Elias C. Aifantis,
Aristotle University of Thessaloniki Polytechnic School, Laboratory of
Mechanics Thessaloniki, GREECE and Center for Mechanics of
Materials and Instabilities, Michigan Technological University,
Houghton, MI; Istvan Groma, Eotvos University Budapest,
Department of General Physics, Budapest, HUNGARY.

Continuum and discrete dislocation dynamics arguments are advanced
leading to reaction-diffusion equations for defect densities. The nature
and physical origin of the gradient and reaction constants are
considered. Applications to pattern formation including dislocation
cells and persistent slip bands are discussed.

11:00 AM Z1.7
DISLOCATION EXHAUSTION DURING PLASTIC
DEFORMATION. Corinne Charbonnier, Olivier Couteau,
Tomas Kruml, Jean-Luc Martin, Ecole Polytechnique Federale,
Department de Physique, Lausanne, SWITZERLAND.

Transient mechanical tests performed along a stress-strain curve yield
valuable information about understanding the dynamics of dislocation
motion. The accurate techniques of repeated relaxations and repeated
creep tests, that we have developed through the years, are briefly
recalled. In the present study they are applied to a variety of crystals,
each one representing a class of deformation mechanisms. It will be
shown that at low temperatures, where dislocation motion is
thermally activated in a rather stable substructure, the decay of the
plastic strain-rate during the transients can be interpreted by taking
into account the exhaustion of mobile dislocations. This exhaustion is
the net result of dislocation multiplication and storage or
annihilation. During the transient, the mobile dislocation density is
considered to be a power function of the velocity (exponent β) and
the mobile dislocation exhaustion parameter can be estimated from
measured β values. The exhaustion of mobile dislocations is estimated
in single crystals of Cu oriented in double slip between 85 and 300 K,

in Ge oriented in single slip between 650 and 850 K, in Ni$_3$Al (with or without additions) in single slip between 80 and 1000 K and polycrystals of binary Ni$_3$Al and TiAl. A fair correlation is found between values of the dislocation exhaustion parameter and the work-hardening coefficient measured on the stress-strain curve prior to the transient: crystals which work-harden significantly exhibit high dislocation exhaustion rates. This is observed when the various materials are compared, but also for a given material at a fixed plastic-strain when the temperature or strain-rate are changed. The differences evidenced between the crystals above are discussed in terms of their peculiar hardening mechanisms: dislocation intersections in Cu, dislocations gliding along parallel planes in Ge with a strong lattice friction, locking mechanisms in the intermetallics.

11:15 AM Z1.8
INTERACTIONS BETWEEN DISLOCATIONS: SIMULATION AND PREDICTION. Ronan Madec, Benoit Devincre, Ladislas Kubin, Laboratoire d'Etude des Microstructures, CNRS/ONERA, Chatillon, FRANCE.

The formation and breaking of junctions between non coplanar dislocations is the main cause of strain hardening in deformed crystals. Atomic as well as mesoscopic simulations have confirmed that the main properties of junctions between perfect or too largely dissociated dislocations can be fully understood within a purely elastic frame. We present here a complete study of the reactions between dislocations on intersecting glide planes in f.c.c. crystals (junction length and strength, bound crossed states, repulsive states) as a function of the initial geometrical parameters. These results are obtained with the help of a recently developed pure-mixed simulation, in which most of the local rules used in previous simulations using the screw-edge model have been relaxed. A very simple model is presented which, like former studies in this domain, is based on the consideration of line energies of straight segments and their elastic interactions. When applied to f.c.c. and b.c.c. crystals, it is shown to have a suprisingly good predictive ability. Among other features, it explains well the origin and properties of the bound crossed sates recently described by Wickham et al. in b.c.c. crystals.

11:30 AM Z1.9
ATOMISTIC-MESOSCOPIC MODELING OF DISLOCATION MOBILITY. Wei Cai, Massachusetts Institute of Technology, Cambridge, MA; Vasily V. Bulatov, Lawrence Livermore National Laboratory, University of California, CA; Jinpeng Chang, Massachusetts Institute of Technology, Cambridge, MA; Joao F. Justo, Instituto de Física da Universidade de São Paulo, São Paulo, SP, BRAZIL; Ali S. Argon, Sidney Yip, Massachusetts Institute of Technology, Cambridge, MA.

We present a powerful, new methodology for quantitative prediction of dislocation mobility through combined atomistic-mesoscopic modeling. Atomistic simulations based on interatomic potentials and first-principles methods are applied to examine core mechanisms of dislocation motion at the angstrom-picosecond scales and to determine the key mobility parameters, such as the double-kink nucleation energies. A mesoscopic kinetic Monte Carlo (kMC) model then incorporates this atomistic input and carries out multiple micron-scale simulation of an entire dislocation line moving through the lattice. This approach is successfully applied to study the dislocation motion in Si and BCC Mo. In the former case, the kMC simulation reveals the essential role of the coupling between the two dissociated partials in understanding the experimentally observed stress dependence of the dislocation velocity, and leads to the clarification of the nature of the longstanding postulate "weak obstacles". In the study on Mo, we apply Molecular Dynamics (MD) simulations to determine the mobilities of short dislocation segments. Such atomistic data are then used to define a local mobility law for kMC simulations of BCC metals featuring cross slip. Besides allowing us to predict temperature and stress dependence of the dislocation velocity, the kMC simulations reveal spontaneous self-pinning, subsequent super jog growth and several other mechanisms whose competition controls the motion of screw dislocations in bcc metals. Also interestingly, our simulations produce a microstructure of debris dislocation loops in the wake of a moving dislocation, in apparently reasonable correspondence with observations. Finally, we discuss an extension of our atomistic-mesoscopic methodology to treatment of the interaction between moving dislocations and point defects and impurities.

11:45 AM Z1.10
THERMALLY ACTIVATED DISLOCATION MOTION: STRESS-DEPENDENT PEIERLS BARRIERS. Nicholas P. Bailey, James P. Sethna, Cornell Univ, Laboratory of Atomic and Solid State Physics, Ithaca, NY; Christopher R. Myers, Cornell Univ, Cornell Theory Center, Ithaca NY.

Dislocation dynamics is an important part of multiscale modeling of materials. As part of a general program for multiscale modeling, we

have studied the motion of a dislocation as a function of stress using atomistic methods. Our focus has been on coding the information obtained from atomistic computations in a suitable functional form for the purpose of modeling dislocations as primitive objects in a larger scale simulation. The functional form is associated with the 'rules' for dislocation motion in the latter simulation. Previously we simulated a dislocation in a two-dimensional material interacting with a Lennard-Jones material. We calculated the velocity in the thermally activated regime (sub-Peierls stress) using transition state theory and the Nudged Elastic Band method for a large range of stresses. This used periodic boundary conditions in the glide direction and had rigid walls on the sides. In the present work we have considered two different types of boundaries. First, continuum boundary conditions where the positions of the boundary atoms are determined by elastic continuum solutions based on multipole expansions centered on the dislocation line. For consistency, one must consider any nonlinear and strain-gradient terms (in the energy expansion) which have the same power-law decay as the multipole terms that are included. Second, in order to facilitate comparisons with electronic structure calculations, we have considered systems with periodic boundary conditions in both directions. This requires four dislocations, two of each sign of Burger's vector such that the force on each vanishes by symmetry. By subtracting off the contribution to the energy from the interactions between all of the periodic images we can compare energies and energy barriers with our single dislocation simulations. For a given interatomic potential these two methods yield the same answers.

SESSION Z2: FRACTURE
Chairs: Huajian Gao and Brad Lee Holian
Monday Afternoon, November 27, 2000
Independence W (Sheraton)

1:30 PM *Z2.1
COHESIVE ZONE MODELS OF INTERFACES AND EXTRINSIC INFLUENCES ON INTERFACE TOUGHNESS. John W. Hutchinson, Harvard University, Cambridge, MA.

Cohesive models employ a traction-separation relation to characterize an interface, requiring specification of a maximum separation stress (an interface strength) and the work of separation. This relation is embedded as an internal boundary condition within a continuum description of the adjoining materials. The models have potential for bridging to the microscopic scale at the interface. Recent applications of this class of models have elucidated important trends on the effects of elastic moduli variations and plasticity in the delamination of thin films and multilayers. This work will be review, and some recent comparisons with a series of experimental studies by R. Dauskardt and co-workers will be featured.

2:00 PM Z2.2
ATOMISTIC-CONTINUUM ANALYSIS OF DECOHESION ALONG INTERFACES. K. Hardikar, R. Phillips, A. Needleman, Div. of Engineering, Brown University, Providence, RI.

The interaction between plastic flow and the actual process of material separation plays an important role in setting the fracture response of materials and bimaterial interfaces. Analyses using cohesive zone model in conjunction with discrete dislocation dynamics have provided much insight into the fracture processes involved in small scale yielding (Cleveringa et. al. J. Mech. Phys. Sol., 48, 2000). In order to simulate realistic fracture behavior, the cohesive zone model, which is used as an input in these simulations, can in turn be derived from atomistic simulations. However, the inherent difficulty in this approach is that the stress levels which arise in atomistic separation process are much higher while the length scales are much smaller than the ones used in higher length scale simulations such as the one in discrete dislocation setting. The present analysis is prompted by the need to resolve this paradox. The analysis involves the study of effective cohesive zone response of an interface in presence of dislocations and interface structure. The cohesive zone model used as an input, is derived from atomistic simulations. Then the analysis is done in a discrete dislocation dynamics setting where the effect of dislocations and interface structure is systematically studied to reveal the way in which it can modulate the response of the interface at a higher length scale.

2:15 PM Z2.3
A PHASE FIELD APPROACH TO CRACK GROWTH DYNAMICS. Lance O. Eastgate, James P. Sethna, Markus Rauscher, Cornell Univ, Laboratory of Atomic and Solid State Physics, Ithaca, NY; Christopher R. Myers, Chuin-Shan Chen, Cornell Univ, Cornell Theory Center, Ithaca, NY.

We present a continuum phase field model for crack propagation. It includes a phase field that is proportional to the mass density and a

displacement field that is governed by linear elastic theory. Generic macroscopic crack growth laws emerge naturally from this model. In contrast to classical continuum fracture mechanics, our model avoids front tracking. The added phase field smoothes the sharp interface, enabling us to use equations of motion for the material (grounded in basic physical principles) rather than for the interface (which often are deduced from complicated theories or empirical observations). The interface dynamics thus emerges naturally. Our model is physically motivated, yet it avoids being specific; it does not focus on a particular material. We incorporate basic properties such as conservation of mass and linear elastic theory. The model is thus generic with respect to fracturing solids, making it easier to identify the basic principles of crack propagation. This project is part of an effort named "Digital Material".

2:30 PM Z2.4
MODELLING OF CRACK GROWTH ALONG A HETEROPHASE INTERFACE WITH A DISCRETE DISLOCATION PLASTICITY METHODOLOGY. <u>E.D. Metselaar</u>, J. Th. M. De Hosson, and E. van der Giessen, Univ. of Groningen, Dept. of Applied Physics and Netherlands Institute for Metals Research, Groningen, THE NETHERLANDS and Micromechanics of Materials Group, Dept. of Mechanical Engineering, Delft University of Technology, Delft, THE NETHERLANDS.

This paper concentrates on an extension of the Discrete Dislocation Plasticity methodology for the simulation of the interaction of a moving crack along a heterophase interface with surrounding lattice dislocations. From classical fracture mechanics it is known that the motion of a crack tip in a homogeneous material is very sensitive to crack tip shielding by lattice dislocations. In a homogenous material a low dislocation density may promote brittle failure whereas at a high density of dislocation sources crack tip blunting without crack propagation can be observed. Therefore the change in the dislocation structure around the crack tip plays a key role in the crack growth process. The growth of an interfacial crack between dissimilar materials is particularly interesting, because the difference in material properties strongly affects the evolution of the dislocation structure. In an effort to understand the dynamical crack growth between dissimilar materials we combined the Discrete Dislocation method and a crack description using dislocation distributions. Important parameters that affect the crack behavior are dislocation mobility, dislocation nucleation and obstacles such as forest dislocations, precipitates etc. The results show that difference in plastic zone size between the two material affect the crack growth process.

2:45 PM Z2.5
MECHANICS OF CRACK BRIDGING UNDER DYNAMIC LOADS. <u>N. Sridhar</u>, B.N. Cox, Rockwell Science Center, Thousand Oaks, CA; C.L. Dunn, Dept of Aeronautics, Massachusetts Institute of Technology, Cambridge, MA; I.J. Beyerlein, Los Alamos National Laboratory, Los Alamos, NM.

Through-thickness reinforcement in the form of fibres, stitches or rods shows great promise for improving delamination resistance in laminated composites. The reinforcement suppresses crack growth by bridging delamination cracks and shielding the crack tip from the applied load. The bridging zones create some unusual characteristics of crack propagation, especially under dynamic loads. It is therefore essential to understand dynamic delamination in the presence of large scale bridging and the micromechanical problem of how the bridging ligament responds to dynamic mixed mode crack displacement. We have formulated and solved a simple model of the dynamic pullout of a generalised fibre from a half-space (e.g., a laminate) and the related problem of dynamic pullout in the bridging zone of a dynamic crack propagating through a composite. The problem is quite subtle - the nature of wave propagation in the presence of frictional forces (or body forces) is not the same as in their absence. In particular, the stress front propagates at speeds less than the longitudinal wave speed in the fibre, if the applied load is a continuously increasing function of time as opposed to discontinuously applied loads. We have derived analytical results for step loads and loads that increase linearly in time, which define the relevant time constants. Inserting values for typical fibre reinforced composites, one finds that dynamic effects will in fact be significant for many crack propagation problems. Using a dynamic traction law rather than a law for static loading is therefore essential in general. We have also formulated fast numerical solutions for general loading cases, which will be required to solve large scale bridging, dynamic crack problems to self-consistency (where the bridging tractions are unknown a priori). We also find that under dynamic loading, analogues of the displacement oscillations found in standard engineering tests under static loading exist, but are now dependent on the crack velocity. Simple models allow regimes of different qualitative crack behavior to be mapped out.

3:30 PM *Z2.6
JAMMING, DEFORMATION, AND FRACTURE IN AMORPHOUS

MATERIALS. <u>J.S. Langer</u> Department of Physics, University of California, Santa Barbara, CA.

I shall summarize recent work by Falk, Lobkovsky and myself in an ongoing attempt to reformulate the theory of plastic deformation in amorphous materials. Our goal has been to produce a theory that is based on atomic-scale deformation mechanisms and, at the same time, provides a unified description of the wide range of phenomena that occur in deformable materials. We have been especially interested in the transition between viscoelastic and viscoplastic behaviors, the dynamics of plastic deformation near advancing crack tips, and the formation of microstructural patterns of shear localization.

4:00 PM Z2.7
MULTISCALE SIMULATIONS OF BRITTLE FRACTURE AND THE QUANTUM-MECHANICAL NATURE OF BONDING IN SILICON. <u>Noam Bernstein</u> and Daryl Hess, Naval Research Laboratory, Center for Computational Materials Science, Washington, DC.

We present multiscale simulations of fracture in silicon that show brittle fracture at low temperature. The simulations use a novel method in which molecular dynamics using the EDIP empirical potential to describe forces on atoms in regions far from the crack tip is dynamically coupled with molecular dynamics using tight-binding to describe forces on atoms at the crack tip. In agreement with experiment, this simulation with a quantum-mechanical description of bonding at the crack tip shows that the crack propagates at the Griffith criterion, and that fracture proceeds through interplanar cleavage with a crack that remains atomically sharp. In contrast, simulations using only empirical potentials show ductile fracture with a blunt crack tip that only propagates at loadings that are several times larger. We compare material parameters that have been proposed as relevant for fracture, such as surface and stacking fault energies, for empirical potentials and tight-binding models. In this context we discuss the origins of the differences between the two types of simulations, and the implications of our results for determining the material parameters that most directly control the nature of fracture. We also explore the effects of temperature and defects, both local and extended, on the nature of fracture.

4:15 PM Z2.8
MESOSCOPIC ANALYSIS OF DISLOCATION BLOCKING INTERACTIONS IN HETEREOEPITAXIAL THIN FILMS. <u>V.B. Shenoy</u>, Brown Univ, Providence, RI; V. Kukta, SUNY-Stony Brook, Stony Brook, NY.

We have used a recently developed mesoscopic dislocation dynamics model to investigate the interactions of strain relieving misfit dislocations and threading dislocation in heteroepitaxial thin films. The model is based on anisotropic elasticity theory supplemented by the explicit inclusion of the separation of perfect dislocations into partial dislocations bounding a stacking fault. We have calculated the strengths of the magnitude activation barriers presented by all the possible blocking intersections as a function of the misfit strain. Comparisons with experimental observations of short-ranged dislocation interactions in SiGe epitaxial films is made.

4:30 PM Z2.9
CRACK BEHAVIOR AT Bi-CRYSTAL INTERFACES: A MIXED ATOMISTIC AND CONTINUUM APPROACH. <u>Arun Pillai</u>, Ron Miller, University of Saskatchewan, Department of Mechanical Engineering, Saskatoon, SK, CANADA.

Interfacial defects like grain boundaries and phase boundaries play an important role in the mechanical behavior of engineering alloys. In particular, these interfaces can influence the fracture properties of a material. The problem of a crack on a bimaterial interface has been well studied from a continuum mechanics point of view. In this work we study this problem at the atomic scale, with the goal of elucidating the effect of varying interatomic interaction on crack behavior and to establish a fracture criterion to predict the behavior of materials. We study a bi-crystal interface crack at the atomic level using the Quasicontinuum(QC) method (V.B. Shenoy, R. Miller, E.B. Tadmor, D. Rodney, R. Phillips, M. Ortiz, Journal of the mechanics and physics of solids, Vol. 47, 1999, p611-p642). The QC formulation incorporates an atomistic constitutive law into a continuum finite element framework. The QC method treats critcal regions like the crack tip atomistically and regions away from the tip as a continuum thereby reducing the degress of freedom and simplifying the application of boundary conditions. The underlying atomistic model used is the Embedded Atom Method. This research has two main objectives. The first is to study the effect of changing the interatomic interaction between the two materials on crack behavior at a bi-crystal interface. The second is to extend existing atomic scale fracture criteria to the bi-crystal case. Fracture criteria have been established based on the surface energy and unstable stacking fault

energy using continuum mechanics to predict the brittle or ductile behavior of cracks (J.R. Rice, Journal of the mechanics of physics of solids, 1992, Vol. 40, p239-271 and J.R. Rice, Z. Suo and J.S. Wang, Metal Ceramic Interfaces, 1990, p269-294). We extend these criteria to similarly predict the behavior of the bi-crystal interface.

4:45 PM Z2.10
MIXED CONTINUUM-ATOMISTIC MODELING OF CRACK GROWTH IN POLYCRYSTALS. Thierry Cretegny, James P. Sethna, Lab of Atomic and Solid State Physics, Cornell University, Ithaca, NY; Erin Iesulauro, Chuin-Shan Chen, Christopher R. Myers, Anthony R. Ingraffea, Cornell Theory Center, Cornell University, Ithaca, NY.

We are developing simulation methods at the mesoscopic scale to study quasi-static crack growth in polycrystals. The grains are considered to be elastoplastic and both intragranular and intergranular fracture are considered. We focus on the description of the grain boundaries in the fracture process and discuss the ways of characterizing their resistance to fracture based on atomic scales studies. The goal is to extract grain boundary properties(when possible as a function of their macroscopic parameters) out of atomistic simulations, summarize and transfer this information across length scales. We consider two approaches to model the behaviour of the grain boundaries at the mesoscopic scale. In the first the fracture toughness as a function of the orientation of the grains is the parameter that contains all the information. The second considers a cohesive zone model, where the microscopic information is summarized in the form of constitutive relations.

<div align="center">
SESSION Z3: DISLOCATION PLASTICITY II
Chairs: John L. Bassani and Sidney Yip
Tuesday Morning, November 28, 2000
Independence W (Sheraton)
</div>

8:30 AM *Z3.1
ATOMISTIC SIMULATIONS OF SIZE SCALE AND STRAIN RATE EFFECTS ON PLASTICITY OF METALS. M.I. Baskes, Structure Property Relations Group, Los Alamos National Laboratory, Los Alamos, NM; M.F. Horstemeyer, Center for Materials and Engineering Sciences, Sandia National Laboratories, Livermore, CA; S.J. Plimpton, Center for Computation, Computers & Math, Sandia National Laboratories, Albuquerque, NM.

We examine the effects of sample size and applied strain rate on single crystal FCC metals. We perform simple shear molecular dynamics simulations using the Embedded Atom Method (EAM) on single crystal nickel ranging from 100 atoms to 100 million atoms and strain rates ranging from 10^7/sec to 10^12/sec to study yield and work hardening. A small number of simulations with different materials (copper and aluminum) and deformation mode (tension and compression) were also conducted. The effects of the large strain rates used in the atomistic calculations was quantified and compared to classical yield models. The increase of flow stress at increasing strain rates is discussed in the context of phonon drag. The results of the atomistic simulations are compared to data from nano-indentation experiments, micro-indentation experiments, small scale torsion experiments, large scale torsion experiments, large scale compression tests, and nanocrystalline compression experiments. This comparison shows that yield varies as $L^{-0.5}$ over eight orders of magnitude in which a length scale parameter, L, is defined by the ratio of volume to surface area. The atomistic simulations reveal that dislocations nucleating at free surfaces are critical to causing microyield and macroyield in pristine material. The atomistic simulations and experimental data show that differences in applied strain rate, temperature, stacking faults (several FCC materials were examined), deformation mode, and crystal orientation on yield and plasticity are small compared to the size scale effect.

9:00 AM Z3.2
SCREW DISLOCATION CORE STRUCTURE, ANNIHILATION AND CROSS SLIP PROCESSES IN FCC Ni. Yue Qi, Alejandro Strachan, Tahir Cagin, William A. Goddard III, California Institute of Technology, Materials and Process Simulation Center, Pasadena, CA.

Using QM-Sutton-Chen many-body potential, we have studied the $<110>/2$ screw dislocation in nickel (Ni) via Molecular Dynamics (MD) simulations. We use a recently developed parallel MD code, which allows us to study systems on the order of 10^5 to 10^6 atoms; this program scales well until 128 processors. We have studied different configurations, namely an isolated dislocation in a cylinder with free surfaces, as well as dipole and quadrupole systems with 3-D periodic boundary conditions. The relaxed structures show dissociation into two partials on {111} planes. The equilibrium separation distance between the two partials is 2.5 nm, which is larger

than the derived value according to experimental data, due to a small stacking fault energy calculated by the force field. The core energy for a dissociated screw dislocation is 0.5eV/b. We also studied motion and annihilation process of opposite signed dislocations with different combinations of dissociation planes, namely when two dislocations dissociated on the same slip plane, on two intersecting slip planes and two parallel slip planes. Peierls potential for each partial has been calculated, and the energy barrier associated in cross slip is studied in detail as well.

9:15 AM Z3.3
YIELD CRITERIA FOR BCC METALS FROM ATOMISTIC SIMULATIONS OF DISLOCATION CORE STRUCTURES. J.L. Bassani, Y. Hu, Dept of Mech Eng & Appl Mech, Univ of Pennsylvania, Philadelphia, PA; K. Ito, Dept of MS&E, Kyoto Univ, Kyoto, JAPAN; J.S. Stölken, Mat Sci & Tech Div, Lawrence Livermore Nat'l Lab, Livermore, CA; V. Vitek, Dept of Mat Sci & Eng, Univ of Pennsylvania, Philadelphia, PA.

For a broad range of crystalline materials non-planar dislocation core structures have a significant effect on macroscopic plastic flow, causing unexpected deformation modes that are strongly influenced by other components of stress in addition to the glide stress on a given slip system and on the sign of stress. In this paper we use atomistic simulations of a screw dislocation in molybdenum and tantalum to determine the influence of non-glide stresses on the critical resolved shear stress required to move the dislocation. The functional form of the Peierls barrier dependence on non-glide stresses is deduced and incorporated into a yield criterion that enters a continuum theory of bcc crystal plasticity. The impact on the yield behavior of single crystals under multiaxial loading conditions is examined.

9:30 AM Z3.4
INTERACTIONS BETWEEN EDGE DISLOCATIONS AND INTERSTITIAL CLUSTERS IN BCC-Fe AND FCC-Cu. Yu N. Osetsky, D.J. Bacon, The Univ of Liverpool, Dept of Engineering, Liverpool, UNITED KINGDOM; B.N. Singh, Risoe National Laboratory, Materials Dept, Roskilde, DENMARK.

Dislocations decorated by clusters of self-interstitial atoms (SIA) and small dislocation loops can play an important role in post-irradiated deformation processes of metals. This feature is of current concern for theoretical and continuum investigations, which aim to understand the mechanisms of the localised plastic deformation that occur in irradiated metals. A major aspect of the problem is related to interactions between dislocation and clusters, and there are usually treated within the framework of elasticity theory. However, it is still not clear whether dislocation-cluster interactions, especially for small clusters at short distance, can be treated accurately by this theory. This issue has to be clarified and requires comparative studies by atomistic simulation and elasticity theory. Here we present a simple example of such a study where interactions between a glissile SIA cluster and an edge dislocation are studied in bcc-Fe and fcc-Cu using both techniques. For Fe we studied the interaction energy of a dislocation with Burgers vector $b = 1/2 < 111 >$ and line direction $< 112 >$ with SIA clusters with the same b situated below the extra half-plane at different distances along the orthogonal $< 110 >$ direction. In Cu the dislocation and clusters had $b = 1/2 < 110 >$ and the dislocation line direction was along $< 112 >$. Interactions with clusters of diameter about 1nm were simulated in both metals. Elasticity calculations were made within the isotropic approximation with parameters estimated from atomistic simulation of the particular dislocation. The results obtained by both techniques are compared and discussed, and conclusions are drawn for the different cases.

10:15 AM *Z3.5
HOW SULFUR TRACES CAN STRONGLY AFFECT THE MECHANICAL BEHAVIOR OF ZIRCONIUM AT INTERMEDIATE TEMPERATURE. Franck Ferrer, Thierry Bretheau, Jérôme Crépin, Laboratoire de Mécanique des Solides, Ecole Polytechnique, Palaiseau, FRANCE; Alain Barbu, Laboratoire des Solides Irradiés, Ecole Polytechnique, Palaiseau, FRANCE.

The addition of some ten ppm of sulfur to α-zirconium and its alloys, has been proved to affect their mechanical behavior in a large range of temperatures (100-500°C) and strain rates (10^{-4}-10^{-8} s^{-1}). For example, the creep rate is divided by 3 at 400°C but the stress sensitivity and the activation energy remain unaffected. On the basis of an inventory of all the possible deformation mechanisms, a multiscale approach, including conventional constant strain rate tensile tests and creep tests, in situ mechanical tests (inside the S.E.M.), T.E.M. observations, and dislocation core structure ab initio calculations, has allowed to precize the controlling mechanisms in that temperature range. For T<200°C, deformation is thought to be controlled by the motion of $<a>$ type screw dislocations submitted to a strong Peierls force due to their non planar core structure. For T>200°C, cross slip or jog dragging (core diffusion) might be the

controlling mechanism. Sulfur affects both the yield stress and the hardening rate. The effect is quite similar to that of strain rate suggesting that sulfur modifies the kinetic but not the nature of deformation mechanisms. Moreover the mode of action of sulfur has been clearly differentiated from the dynamical hardening mechanism considered as pertinent to explain the action of oxygen. We propose that sulfur segregates into the screw dislocation cores (the calculated interaction energy is favorable) and modifies its structure resulting in a higher Peierls force at low temperatures and in a modification of core diffusion or of cross slip facility at higher temperatures.

10:45 AM Z3.6
INTERACTIONS BETWEEN HYDROGEN AND DISLOCATIONS IN ALUMINUM: A THEORETICAL STUDY. Gang Lu, Nicholas Kioussis, California State University Northridge, Dept. of Physics, Northridge, CA.

The understanding of the interactions between H and dislocations in metals is of considerable importance due to the influence of these effects on plastic flow and H mobility. In this paper we employed the semidiscrete generalized Peierls-Nabarro model to study the core properties of various dislocation in Al with and without H impurity. The generalized stacking fault energy surfaces entering the model were calculated from the density functional theory with a large supercell to model the low concentration of the H impurity (less than 5 at. %). Various dislocation core properties, including core width, dissociation into partials, energetics and Peierls stress were calculated with and without the H impurity and the interactions between the H and dislocations were then revealed. In special, we calculated the binding energy between H and dislocation cores and examined the dependence of the binding energy on the dislocation characters. More importantly we were able to obtain the separate energy contributions (elastic and misfit) from the interactions between the H and dislocations. The atomic core structures for the various dislocations were compared with and without the H impurity. The two opposing effects of H on the motion of dislocations, pinning effect vs. H-enhanced local plasticity were discussed based on the calculated Peierls stress.

11:00 AM Z3.7
HYDROGEN EMBRITTLEMENT IN ALUMINUM: A FIRST PRINCIPLES INVESTIGATION. Ickjin Park[2], Olivier Politano[2], Daniel Orlikowski and Efthimios Kaxiras[1,2]. [1]Department of Physics, Harvard University, Cambridge, MA. [2]Division of Engineering and Applied Sciences, Harvard University, Cambridge, MA.

We present the numerical results of a first principles investigation of interstitial hydrogen impurities in aluminum. In general, the addition of hydrogen to an aluminum system can shift the intrinsic behavior to be more brittle in character. To further understand this, we have performed energetic calculations of aluminum systems with varying concentrations of hydrogen impurities in a *crack* geometry. Specifically, for such systems the generalized separation and traction curves along $[\bar{2}11]$ in the (111) surface are calculated. The results indicate that hydrogen impurities induce a dilational strain in the aluminum lattice. Moreover, we find, that there is a strong dependence of the slip barrier on the applied tensile strain. By increasing the hydrogen coverage, the effective stacking fault energy (SFE) can be significantly reduced, indicating enhanced plasticity for dislocation mobility. Also, the implications of this investigation for possible mechanisms of hydrogen embrittlement are discussed.

11:15 AM Z3.8
ATOMIC SCALE SIMULATION OF THE EFFECT OF HYDRO-GEN ON DISLOCATIONS. C. Domain, Département Etude des Matériaux, EDF-DRD, Moret Sur Loing Cedex, FRANCE; A. Legris, Laboratoire de Metallurgie Physique et Genie des Materiaux, UMR 8517, Universite de Lille 1, Villeneuve d 'Asq, FRANCE.

In nuclear power plants, cladding made of Zr based alloys subjected to the corrosion by the primary coolant undergo hydrogen pick-up. Hydrogen absorption and diffusion, in solution but also hydrides modifies the mechanical properties of the cladding materials in service and storage conditions. In zirconium the deformation is partially controlled by the intrinsic screw dislocations mobility [1]. The core structure spreads in the prismatic plane with a basal contribution that is responsible for the relatively low dislocation mobility. It is the objective of this work to address the dislocation core-hydrogen interactions that can not be described within the framework of the linear elasticity theory. We have performed first principle calculations, based on the density functional theory to determine the zirconium-hydrogen interactions. As far as plasticity is concerned, we have focused on the energetics of a screw dislocation core-hydrogen interactions and also on the modifications of the prismatic and basal gamma surfaces induced by hydrogen. Furthermore, in order to investigate possible influences on the dynamic strain ageing behaviour, the hydrogen-oxygen interactions in solid solution were determined. [1] B. Legrand, Phil. Mag. B **49 (1984) 171-184.**

11:30 AM Z3.9
MOLECULAR DYNAMICS SIMULATION OF DISLOCATION MOTION IN BCC MOLYBDENUM. Jinpeng Chang[1], Wei Cai[1], Vasily V. Bulatov[2], Sidney Yip[1]. [1]Massachusetts Institute of Technology, Dept of Nuclear Engineering, Cambridge, MA. [2]Lawrence Livermore National Laboratory, Livermore, CA.

The calculation of single dislocation velocity as a function of temperature and stress is an important step towards the understanding of single crystal stress-strain constitutive relationship in terms of dislocation theory. In this work, the motion of initially relaxed single dislocations (both edge and screw) in BCC Mo with b=1/2⟨111⟩ on (112) plane under constant shear stress is studied by Molecular Dynamics using the Finnis-Sinclair potential with periodic boundary condition(PBC). The effect of PBC is calculated using linear elastic theory to determine the optimal simulation settings. The dynamic pathway of the dislocation line is extracted by analyzing the spatial disregistry between adjacent atom rows. The motion of single edge dislocation is observed to involve frequent double-kink nucleation but few kink migration; moreover, edge dislocation velocity does not change with an initially created kink. These suggest a much higher activation energy of kink migration than kink nucleation. This finding would be tested by further MD and ab-initio studies. Dislocation velocity as a function of temperature and stress has been determined in studied regions where dislocation motion is governed by phonon drag. Similar analysis are undertaken for kink mobility on screw dislocations. Furthermore, hyperdynamics simulation will be implemented to extend the time scale to simulate low-stress low-velocity regime where dislocation motion is mostly thermally activated. In parallel, our atomistic calculations will be coupled with kinetic Monte Carlo(kMC) simulations where dislocation motion is modeled by sampling the stochastic sequence of double-kink nucleation and kink migration events, with their rates determined by activation energies, for which some of the first principles are already available. The results of MD and kMC will be compared, which has not been done by anyone. We believe that this would be essential to validate the statistical assumptions of Monte Carlo modeling of dislocation motion.

11:45 AM Z3.10
FIRST PRINCIPLES SIMULATIONS OF ISOLATED SCREW DISLOCATIONS IN BCC METALS. C. Woodward*, S.I. Rao*, Air Force Research Laboratory, Wright-Patterson AFB, OH. *Materials and Processing Div., UES, Inc. Dayton, OH.

The equilibrium core structure of isolated a/2<111> screw dislocations are calculated using a first principles pseudopotential planewave method within the Local Density Approximation of Density Functional Theory. The long range strain field of the dislocation is treated using a variation of the recently developed lattice Greens Function Boundary Condition method. This flexible boundary method allows the dislocation to be contained in a very small simulation cell without compromising the fidelity of the final core configuration. Supercells of 168 and 270 atoms are used to evaluate the local screw and edge displacements of the a/2<111> screw dislocation in Mo and Ta. These results are contrasted with previous results from atomistic and dipole array calculations. We find that the isolated screw dislocations are evenly spread onto three conjugate (110) planes for both Mo and Ta. The twinning/anti-twinning anisotropy is calculated in Mo by applying a pure glide stress on the (112) plane. In these simulations the dislocation always moves on a {110} plane. The lattice friction stress to move a straight screw dislocation on the (112) plane in the anti-twinning and twinning sense is estimated at 0.025μ and 0.0125μ respectively. This is in good agreement with parallel atomistic simulations and experimental measurements of the slip asymmetry.

SESSION Z4: SIZE EFFECTS IN PLASTICITY –
INDENTATION AND THIN FILMS
Chairs: Efthimios Kaxiras and William D. Nix
Tuesday Afternoon, November 28, 2000
Independence W (Sheraton)

1:30 PM *Z4.1
MULTISCALE MODELING OF INDENTATION RESPONSE DUE TO MICROSTRUCTURE GRADIENTS AND ELECTRICAL-MECHANICAL COUPLING. Subra Suresh, Massachusetts Institute of Technology, Dept of MS&E, Cambridge, MA.

Modelling the effects of multiscale deformation processes on micro- and nano-indentation will be considered in this presentation in the context of two specific classes of materials: (a) those in which gradients in properties exist at the indented surface, and (b) those in which the deformation mechanisms are strongly influenced by electrical /mechanical coupling. The former class includes materials

which comprise gradients in composition (as, for example, due to case hardening), defect density (e.g., gradients in dislocation density beneath the indented surface), or elastic moduli (ion implantation). The latter class primarily deals with piezoelectric ceramics, wherein experimentally verifiable connections will be made between the imposed mechanical loads and the ensuing electric response or vice versa. Results of analytical and computational modeling at different length scales will be presented for both cases to illustrate how the indentation response is drastically altered from that seen in purely mechanical systems with spatially homogeneous composition. Attention will also be devoted to the occurrence of distinct transitions in deformation mechanisms across widely differing size scales of indentation, spanning the nanoindentation to the macroindentation regime.

2:00 PM Z4.2
MODELING OF THE INDENTATION OF PLASTICALLY GRADED SURFACES. <u>Antonios E. Giannakopoulos</u>, Subra Suresh, Massachusetts Institute of Technology, Department of Materials Science and Engineering, Cambridge, MA.

The measurement of local mechanical response of materials with gradients in plastic properties is a topic of considerable technological importance, especially in situations where only small material volumes are available for testing. Examples of such applications invoke multiple miscrostructural and mechanical length scales and include graded thin films in strained layer epitaxy for optoelectronic applications, case hardened steels used in structural components, ion-implanted surfaces used in microelectronic devices and laser-treated or work-hardened surfaces with gradients in dislocation density. A promising technique for mechanical measurements in such applications is depth-sensing instrumented indentation, because the variation with depth of mechanical properties such as yield strength and strain hardening plays an important role in the indentation response of graded surfaces. We present an analysis of sharp indentation response of some general classes of plastically graded surfaces. The variation of the plastic properties are further correlated with spacial variations of composition or dislocation densities. The predictions of the analysis are compared with finite element simulations and with available experimental observations.

2:15 PM Z4.3
COMPUTER SIMULATION OF NANO-INDENTATION INTO POLYMER FILMS. <u>Dieter W. Heermann</u>, Institut für Theoretische Physik, Universität Heidelberg, Heidelberg, GERMANY.

In this contribution, I will report on computer simulations of nano-indentation into amorphous polymer films. I will concentrate on the initial, kinetic stage of the indentation process and give results for the motion of the indenter, the deformation field of the polymer film, the stress field, and the field of total monomer energy. I will propose an effective coefficient as a new measure for the resistivity of a surface against indentation. Its value can be determined in an experiment with constant indentation velocity.

2:30 PM Z4.4
INDENTATION MODELING OF PARTICLE-CONTAINING MATERIALS: INVALIDITY OF THE CONTINUUM-BASED HIERARCHICAL APPROACH. <u>Yu-Lin Shen</u>, Ying Long Guo, Univ of New Mexico, Dept of Mechanical Engineering, Albuqueruqe, NM.

In modeling mechanical properties of heterogeneous materials across length scales, a hierarchical approach is frequently adopted: microstructural features are first included in the small-scale model, from which effective properties of the material are extracted and subsequently used as input parameters for analyses at a larger scale. For instance, modeling the overall stress-strain response of a multiphase material is amenable to such type of approach. In this study we seek to explore the validity of this methodology in continuum-based indentation modeling. We focus on materials consisting of hard particles embedded within a soft matrix. A model composite system containing particles and matrix is constructed and the overall stress-strain response is modeled. The stress-strain response then serves as the inherent properties of a homogeneous material subject to indentation modeling. In a parallel fashion, indentation modeling is directly conducted on the two-phase composite system. Although the two-phase system and the homogeneous system possess exactly the same overall stress-strain behavior, the two-phase system consistently shows a significantly harder response under indentation, even when the particle size is much smaller than the indent size. This is due to the localized nature of indentation-induced deformation: the concentration of hard particles is increased directly underneath the indentation. This means that treating the material as a homogeneous continuum, though at a large scale compared to the microstructural feature size, is not a valid approach for indentation modeling. Indentation tests on discontinuously reinforced metal matrix composites are also

performed, and the experimental results support the numerical findings.

3:15 PM *Z4.5
WHAT'S IN A NANOINDENTATION LOAD-DISPLACEMENT CURVE? <u>George M. Pharr</u>, The University of Tennessee, Dept of MS&E, Knoxville, TN and Oak Ridge National Laboratory, Metals and Ceramics Division, Oak Ridge, TN; Alexei Bolshakov, Baker-Hughes Inteq, Houston, TX; Haitao Song, Licenergy Inc, Houston, TX.

Measurement of mechanical properties at small scales by load and depth sensing indentation methods, often referred to as nanoindentation, is based on load-displacement data obtained as an indenter is driven into and withdrawn from the material. For sharp indenters like the Berkovich three-sided pyramid used frequently in nanoindentation studies, indentation loading curves are usually well-described the simple power law relation $P = Bh^2$, where P is the load, h is the penetration depth, and B is a constant related to the geometry of the indenter and the elastic and plastic properties of the material. During unloading, the relation $P = A(h-h_f)^m$ is a good representation of experimental behavior, where h_f is the final depth after complete unloading, and A and m are material constants. The power law exponent, m, for the unloading curve is not fixed at an integral value, but varies from material to material in the range m=1.2-1.6. Simple models based on elastic-plastic indentation by a rigid cone are presented which give a physical explanation for these behaviors. The models also provide a means by which the material constants appearing in the relations can be related to more fundamental material properties such as the elastic modulus and yield strength.
*Research at the Oak Ridge National Laboratory SHaRE User Facility was sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

3:45 PM Z4.6
SPACE-TIME ANALYSIS OF PROPAGATING PORTEVIN–Le CHATELIER DEFORMATION BANDS. <u>Peter Hähner</u>, Technische Universität Braunschweig, Inst. f. Metallphysik und Nukleare Festkörperphysik, Braunschweig, GERMANY.

The serrated yielding associated with the Portevin–Le Châtelier (PLC) effect which represents the most prominent example for plastic instability due to strain-rate softening, is attracting continuous interest from the technical (metal forming), metal physical (dynamic strain ageing) and theoretical (nonlinear dynamics) points of view. After a brief review of previous phenomenological models incorporating a negative strain-rate sensitivity of the flow stress, a new model the PLC effect is presented which is explicitly based on the kinetics of dynamic strain ageing as the microphysical origin of strain-rate softening instability. By considering the additional activation enthalpy for dislocation unpinning from the solute clouds as an internal dynamical variable of the model, a balance between the solute accumulation in the dislocation cores due to strain ageing and the solute depletion by dislocation activation is formulated. This dynamics is coupled to the plastic flow behaviour which is affected by strain hardening and by the mechanical response of the tensile machine. The model incorporates a spatial coupling due to the cooperative dislocation interactions which are closely related to the appearance of strain-rate softening instability. Hence, the model allows for relating plastic instability to spatio-temporal localization of plastic flow (deformation banding). In addressing the question of the selection of the PLC band speed, analytical results are derived for the PLC band parameters (band velocity, width and strain), which are in fine quantitative agreement with recent experimental results. Moreover, transitions between various types of PLC bands (uniformly propagating bands of Type A, discontinuously propagating bands of Type B, and random strain bursts of Type C) are analysed and compared to experimental findings. Finally, computer simulation results of the model are presented revealing the complex space–time dynamics of PLC banding as confirmed experimentally by recent laser extensometer investigations.

4:00 PM Z4.7
THE CONNECTION BETWEEN TEMPORAL AND SPATIAL INHOMOGENEITY IN SHEAR DEFORMATION: A COMPUTER SIMULATION EXAMPLE. <u>Xue Min Gu</u>, Yong Qian Sun, University of Illinois at Urbana-Champaign, Dept of Materials Science and Engineering, Urbana, IL.

There is an intrinsic connection between spatial and temporal inhomogeneity in an unstable plastic shear. In the present work, this connection is studied by kinetic Monte Carlo simulations of plastic instability due to dynamic strain ageing. The results of the simulation indicate that temporal inhomogeneity or serrations on stress-strain curves, known as Portevin-Le Chatelier effect, is strongly related to

spatial inhomogeneity of strain localization. The temperature and strain rate domain in which temporal and spatial inhomogeneity exist are identified.

4:15 PM Z4.8
MECHANICAL AND MESOSTRUCTURAL APPROACH OF LOCALIZATION. Thierry Hoc, Colette Rey, Ecole Centrale Paris, MSSMAT, Chatenay Malabry, FRANCE; Eric Labbe, IFTS, Charleville Mezieres.

In polycrystals, localization of strain i.e. sets of narrow bands carrying a large amount of plastic deformation, corresponds to an instable phenomenon, frequently observed during cold forming processes. In order to simulate such processes, the localization of a mild steel submitted to a sequential loading paths is investigated at macroscopic, mesoscopic and microscopic scales. Experimental tensile tests were performed in a scanning electron microscope, using microgrids and crystalline orientation methods and gave a set of data on local strain and rotation fields evolution at the scale of the grains. The experimental results show that the localization depend mainly on the microstructural anisotropy and that macroscopic instabilities are composed by a set of parallel mesobands, few micrometers width, crossing grain boundaries. Comparisons with observations performed on iron and copper single crystals tensile tested in the same conditions, point out peculiar mechanisms to post bifurcation stage. A crystalline model using a finite element code is proposed. The model allows to take into account the morphology of grains and the crystalline orientations. The effects of interactions between adjoining grains were then emphasized and local internal stresses due to strain incompatibility were computed. The crystalline approach was based on a description of dislocation densities evolution on the different slip systems. The main advantage of this model is to give a description of the microstructure evolution and by return of anisotropy evolution. The model gives access to different physical parameters acting on localization bands leading to a better understanding of this phenomenon. These results are compared to those obtained by a mechanical model based on the Asaro's criteria of bifurcation developped for a planar single crystal. A discussion on the slop of the stress-strain curve is conducted.

4:30 PM Z4.9
COARSE SLIP BANDS IN SINGLE- AND POLY-CRYSTALLINE SOLIDS OF AN ALUMINUM ALLOY. Seung-Yong Yang, Xianghong Li, Wei Tong, Yale University, Department of Mechanical Engineering, New Haven, CT.

It is well known that plastic deformation of single crystals becomes highly nonuniform at relatively small plastic strains, especially in metal alloys. One of the examples is the appearance of coarse slip bands under monotonic uniaxial stressing of a crystal. Triggering of such nonuniform plastic flows has been analyzed in the past mainly in term of secondary slips and non-Schmid effects in a framework of rate-independent crystal plasticity formulation. Here we present a unified treatment of growth and evolution of coarse slip bands in both single and poly-crystalline solids of an aluminum alloy over a range of length and time scales with a focus on the interaction of dislocations and alloying elements in the alloy and its role in setting the hardening rules on individual slip systems of the aluminum crystal. A rate-dependent crystal plasticity formulation which accounts for such interactions will be used to analyze the formation of coarse slip bands and macroscopic shear bands in aluminum under both single- and multiple-slip conditions. Results of our analysis are compared with existing experimental data.

4:45 PM Z4.10
A NEW X-RAY WINDOW ON DEFORMATION MICRO-STRUCTURES. L.E. Levine, G.G. Long and R.J. Fields, NIST-MSEL, Gaithersburg, MD.

New ultra-small-angle X-ray scattering (USAXS) facilities at 3rd generation >synchrotron sources enjoy an additional 1 to 3 decades of X-ray brilliance over 2nd generation instruments, and can now quantify microstructural features from 3 nm to 8 micrometers in size. These developments offer exciting possibilities for further exploration of dislocation and other deformation microstructures. To the portfolio of existing techniques we now add a promising experimental window, USAXS imaging, in which high angular resolution images are acquired at scattering vectors related to the observed microstructures. In the first experiments using this ultra-sensitive technique, the spatial arrangements of creep cavities in mildly deformed polycrystalline copper were observed on many length scales, and the results were correlated with the statistically-significant size distributions derived directly from a USAXS analysis. Many of the features observed in the USAXS images cannot be observed using other existing experimental techniques.

SESSION Z5/Y6: JOINT SESSION
STRAIN LOCALIZATION AND DISLOCATION
PATTERNING
Chairs: Michael Zaiser and Ladislas P. Kubin
Wednesday Morning, November 29, 2000
Independence (Sheraton)

8:30 AM *Z5.1/Y6.1
SPATIAL DISTRIBUTIONS OF DISLOCATION STRUCTURES FROM MILLIMETERS TO NANOMETERS. Darcy A. Hughes, Center for Materials and Engineering Sciences, Sandia National Laboratories, Livermore, CA.

The key element describing dislocation structures formed during cold deformation in medium to high stacking fault energy fcc metals is a cell block. A cell block is composed of cell block boundaries (flat extended geometrically necessary boundaries, GNBs) and cell boundaries (short incidental dislocation boundaries, IDBs). Small lattice rotations occur across the IDBs, whereas, much larger and significant lattice rotations are observed from one cell block to its neighbor. This difference is in accord with the difference in slip patterns between neighboring cellblocks. The spacing of both types of boundaries decreases monotonically with increasing strain while the misorientation angles across them increase with increasing strain. For example, depending on the deformation conditions and material, the size of a cell block can range roughly from 10x100x100 micrometers to 10x100x100 nanometers. Misorientation angles can range from 1 to 62.8 degrees. Thus the cell blocks accumulate a record of the slip pattern. Mapping the distribution of the cell block parameters, either across a grain in a polycrystal or along a deformed single crystal or bicrystal, can be used to explore the larger scale effects of grain orientation; grain boundaries; as well as the constraints arising from the deformation boundary conditions such as friction, sample grips, and test platens. This is illustrated by comparisons dislocation structures that form in single crystals, bicrystals and polycrystals as a function of strain.
This work was supported by the U.S. DOE Office of Basic Energy Sciences, Division of Materials Sciences under contract no. DE-AC04-94AL85000.

9:00 AM *Z5.2/Y6.2
DEVELOPMENT, SCALING AND EVOLUTION OF DISLO-CATION CELL SUBSTRUCTURES. Elizabeth A. Holm, Sandia National Laboratories, Albuquerque, NM; Richard A. LeSar, Los Alamos National Laboratory, Los Alamos, NM; Mark A. Miodownik, Dept. of Mechanical Engineering, University College Dublin, IRELAND.

The development of a dislocation cell substructure has been observed in a wide variety of plastically deformed metals. Both cell size and cell boundary misorientation distributions follow apparently universal scaling functions, and the average size and misorientation correlate with the total plastic strain. Analysis of random dislocation arrays shows such scaling behavior; however, there is a quantitative discrepancy between theory and experiment. Monte Carlo energy minimization simulations for dislocation array evolution indicate cell formation with cell orientations more narrowly distributed than for a random array. The effect is present in two-dimensional simulations of edge dislocations and becomes more dramatic in three-dimensional systems. The narrowing of the cell orientation distribution reflects a competition between entropy (favoring randomness and a Gaussian cell orientation distribution) and enthalpy (favoring minimization of cell boundary energy via small misorientations). When this competition is included in the analytical theory, the experimentally observed scaling function is produced. Furthermore, this scaling is found in a variety of systems exhibiting a competition between randomness and order. The universal misorientation distribution, along with appropriate boundary motion laws, is incorporated in a cellular automaton model for microstructural evolution, and cell size scaling is observed. Evolution of the cell substructure occurs by uniform recovery, with self-similar cell size and misorientation distributions characterized by a continuously increasing average cell size and a continuously decreasing average misorientation. Abnormal cell growth, which would indicate a recrystallization nucleation event, does not occur.

9:30 AM Z5.3/Y6.3
COMPUTER SIMULATIONS OF DISLOCATION CELL STRUCTURE EVOLUTION. Mark A. Miodownik, Department of Mechanical Engineering, University College Dublin, Belfield, Dublin, IRELAND; Elizabeth A. Holm, Sandia National Labs, Albuquerque, NM.

The annealing behaviour of dislocation cell structures is explored using a 3D cellular automaton model of dislocation boundary evolution. A Monte Carlo technique is used to construct the initial dislocation cell structures. These are statistically equivalent to

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experimentally measured deformation structures. Cell boundaries contain both geometrically necessary and redundant dislocations and are thus in a non-equilibrium state at the beginning of the simulation. As a result of dislocation climb and recombination the redundant dislocation content of the boundaries decreases during the simulation. This recovery process alters the boundary energy and mobility of the dislocation cell boundaries. Curvature driven cell boundary migration takes place concurrently with this recovery process and coarsens the cell structure. Two distinct regimes of behaviour are identified. These are defined critically by the rate of boundary recovery. The first is normal cell growth in which the average cell boundary misorientation decreases with time and cell size increases uniformly. In the second regime an incubation period of microstructural stagnation is followed by abnormal cell growth, in which cells with high misorientation boundaries migrate and consume all other cells. It is important to note that these abnormal cells do not need to be artificially introduced but occur naturally as outliers in the dislocation cell distribution. This process strongly resembles the early stages of recrystallization. We discuss the crucial role played by redundant dislocations and report on experiments to measure their density in deformed aluminium single crystals.

9:45 AM Z5.4/Y6.4
DISLOCATION PATTERNING AND VORTEX CHANNELING IN THE XY MODEL. Robin L.B. Selinger and Brian B. Smith, Catholic Univ. Physics Dept., Washington, DC.

To understand how dislocations form ordered structures during the deformation of metals, we study the patterning of defects in a related but simpler system, the XY rotator model with twisting boundary conditions. While highly idealized, this model provides useful insight into the basic phenomena of plasticity. Vortices in the XY model are close analogs of screw dislocations, and the applied twist rate is analogous to an applied shear strain rate. Simulations of the model in 2-D show the spontaneous formation of vortex channels, where each channel is a narrow strip along which defects flow at high density, as in a shear band. Channels are separated by wide defect-free regions, and after initial formation the channel spacing widens gradually through a coarsening process, reaching an apparent equilibrium value which varies with both temperature and strain rate. Both channel spacing and overall defect density obey scaling relationships with the applied strain rate. We explain this pattern formation process as a phase separation between ordered and disordered phases of the 2-D XY system, at temperatures well below the Kosterlitz-Thouless transition. The introduction of a crack and bond-breaking rules into the model reveals a brittle/ductile transition with temperature and strain rate. Preliminary results for the 3-D XY rotator model under twisting boundary conditions also show coalescence of vortex lines/loops into shear bands. Potential applications include studies of the size effect and strain gradients in plasticity, and testing the Khantha-Pope-Vitek theory of the brittle-ductile transition. This model may also describe the channeling of vortices in type II superconductors.

10:30 AM *Z5.5/Y6.5
DISLOCATION PATTERNING: STOCHASTIC APPROACH TO MESOSCALE MODELING. Peter Hähner, Technische Universität Braunschweig, Institut für Metallphysik und Nukleare Festkörperphysik, Braunschweig, GERMANY.

Plastic deformation by dislocation glide is known to be associated with the spontaneous formation of mesoscopic patterns of various types, e.g. cellular dislocation structures during unidirectional deformation and quasi-periodic persistent slip band structures during cyclic deformation. While it is recognized that dislocation patterning represents a dissipative far-from-equilibrium process, theoretical modeling of those phenomena is complicated by the long-range nature of dislocation interactions inducing collective dislocation behaviour on a mesoscopic scale. In this paper the problem is addressed using a stochastic approach with random fluctuations acting on the evolution of the dislocation ensemble. The intensity of the fluctuations is determined self-consistently from dynamic dislocation interactions and, hence, reflects correlated dislocation motion. It is shown that those fluctuations may induce dislocation patterns by stabilizing non-uniform dislocation distributions. Microstructure-based models are presented for unidirectional and cyclic plastic deformation. In the first case fractal dislocations distributions corresponding to hierarchically organized dislocation cell structures are obtained, while in the latter case a decomposition into dislocation-rich walls or veins and depleted channels is found, which are associated with the formation of persistent slip bands and matrix structures. The results are compared to experimental observations in single-crystalline fcc metals. The close agreement points at the importance of collective dislocation effects in the self-organization of those structures.

11:00 AM Z5.6/Y6.6
STATISTICAL PROPERTIES OF DISLOCATION ASSEMBLIES.

I. Groma, Eötvös University Budapest, Department of General Physics, Budapest, HUNGARY.

It is well known that during the plastic deformation of crystalline materials the dislocation distribution does not remain homogeneous. In spite of the increasing experimental and theoretical activity on this field we are far from the understanding of these typically self organizatory phenomena. A possible approach for the modeling of these pattern formation processes is to investigate the collective behavior of systems consisting of individual dislocations by computer simulation. However, because of the long range character of the dislocation interaction the direct numerical integration of the equations of motion of dislocations are very computation expensive restricting considerable the affordable dislocation number or simulation volume. The aim of the investigations presented in the paper is to to overcome this restrictions by taking into account the statistical properties of the dislocation assembly. In the first part of the paper it is shown that the individual (micro scale) and the continuum (meso scale) approaches can be linked through the construction of a hierarchy of evolution equations of the different order dislocation distribution functions. By neglecting the dislocation-dislocation correlations a self-consistent field description is derived which can be considered as a zero order approximation. In the second half the behavior of a system of straight parallel dislocations is investigated. It is found by numerical simulation that the internal stress τ created by the dislocations has a stochastic component. In order to describe this stochastic character the form of the probability distribution function of the internal stress is determined. It is shown that the mean value of the distribution function is the self-consistent field created by the dislocation, and the distribution function decays with $1/\tau^3$.

11:15 AM Z5.7/Y6.7
DISLOCATION MULTIPLICATION IN GERMANIUM: COMPARISON OF EXPERIMENTAL AND SIMULATION RESULTS. C. Charbonnier, T. Kruml and J.L. Martin, Ecole Polytechnique Federale, Department de Physique, Lausanne, SWITZERLAND.

About dislocation multiplication and covalent crystals and the associated yield-point, several questions remain open. A study of this phenomenon is underway on Ge single crystals oriented in single glide. Monotonous compression tests are performed together with transients (relaxation and creep tests) at various temperatures (650 - 850 K) and strain-rates (10^{-5} to $4.10^{-4} s^{-1}$). Dislocation structures are observed in the transmissioon electron-microscope. The conditions of chemical polishing of the lateral faces have been defined so as to remove surface defects, the presence of which affects the height of the yield-point. The transients are performed before the upper yield-point and after the lower yield-point for comparison. At similar stresses, the corresponding deformation-rate is observed to be smaller in the former part of the stress-strain curve as compared to the latter. This corresponds to a lack of mobile dislocations at the onset of deformation. The activation parameters of dislocation mobility are determined after the lower yield-point and correspond to a lattice friction mechanism. They are used to analyze the measurements before the upper yield-point, in an attempt to obtain experimental data about mobile dislocation densities as a function of time. The values of the latter parameter will be compared with those predicted from 3D simulations of Frank Read sources in a covalent material (Si) performed by Moulin, Condat, Kubin (Acta Mater. 1999).

11:30 AM Z5.8/Y6.8
SIMULATION OF DISLOCATION CELL STRUCTURES. Benoit Devincre, Diego Gomez-Garcia, Ladislas P. Kubin, LEM, CNRS-ONERA, Chatillon, FRANCE.

It has been known for a long time that dislocation cells are formed at low and medium temperatures in FCC single crystals deformed into stage III, or from the onset of plastic flow in multislip conditions. In BCC crystals cell structures are also formed in conditions of stain and temperature such that the interactions between dislocations prevails over the lattice friction. The objectives of dislocation dynamics simulations in this domain are to reproduce dislocation cell formation, define the leading mechanisms that contribute to it and, possibly, understand the stress dependence of the cell dimensions (the so-called similitude principle). Results are shown of a 3-D simulation of FCC crystals deformed in multislip conditions at room temperature. Dislocation cells are formed at strains of the order of 0.5%. The role of various dislocation mechanisms has been cleared out by switching them on and off one by one. This leads to the conclusion that dislocation storage and the initial steps of the formation of cell structures mainly depend on short-range mechanisms and interactions. In contrast with what is usually thought, long range elastic interactions do not contribute significantly to the bifurcation from uniform to non-uniform dislocation microstructures. More specifically, short-range interaction stresses favor cross-slip events that

lead to storage of debris and stable dislocation configurations. The latter, together with stable dislocation locks, serve as anchoring points for the formation of dislocation cells. Once the latter are formed, a pattern of long-range stresses is established that enhances their further development. Attempts to investigate the origin of the similitude principle are discussed with the help of a 2.5-D simulation that mimics in 2-D the three-dimensional mechanisms described above.

11:45 AM Z5.9/Y6.9
STRAIN GRADIENTS AND PATTERNING OF PLASTIC FLOW. John L. Bassani, Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA.

Localized deformation during plastic flow of crystalline metals commonly leads to microstructural patterning. One of the most widely observed patterning is the lamella microstructure associated with coarse slip. We have shown that fine secondary slips that contribute significantly to overall hardening behavior also play an important role in the nucleation and stabilization of such localized modes of deformation. These secondary slips can also control patterning, e.g. thickness and spacing of coarse slip bands, through the effects of lattice incompatibility. In continuum theory the crystal lattice is assumed to distort only elastically, while generally the elastic deformation itself is not compatible with a single-valued displacement field. A simple gradient (nonlocal) theory is discussed in which incompatibility only enters the instantaneous hardening relations. As a result, the classical bifurcation calculations relevant to shear localization are preserved for rate-independent behavior. Predictions for patterning of localized deformation using this theory are promising.

SESSION Z6: ATOMISTICS
Chairs: Peter Gumbsch and Kyeongjae Cho
Wednesday Afternoon, November 29, 2000
Independence W (Sheraton)

1:30 PM *Z6.1
BOND-ORDER POTENTIALS: BRIDGING THE ELECTRONIC TO ATOMISTIC MODELLING HIERARCHIES. David Pettifor, Ivan Oleinik and Duc Nguyen-Manh, Oxford Univ, Dept of Materials, Oxford, UNITED KINGDOM.

Novel analytic bond-order potentials (BOPs) are derived for atomistic simulations by coarse graining the electronic structure within the orthogonal two-centre tight-binding (TB) representation. We show that these BOPs allow the concept of single, double, triple and conjugate bonds in carbon systems to be qualified, so that they provide the first 'classical' interatomic potentials that handle both structural differentiation and radical formation naturally within their remit. Finally, we show that this recently-developed BOP formalism allows us to derive explicit, analytic expressions for the environmental dependence of the TB bond integrals, applying the theory to the high-temperature intermetallics alloys $MoSi_2$.

2:00 PM Z6.2
BOND-ORDER POTENTIALS FOR ATOMISTIC STUDIES IN Ti-Al ALLOYS. S. Znam, V. Vitek, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA; D. Nguyen-Manh and D.G. Pettifor, Department of Materials, University of Oxford, Oxford, UNITED KINGDOM.

A variety of LDA based ab-initio calculations indicate that the bonding in Ti-Al alloys is not purely metallic and that the covalent component of bonding is significant. However, studies of extended defects have been made ubiquitously using central-force potentials. The method in which the required covalent character of bonding is included is the tight-binding method and recently it has been reformulated in terms of Bond-Order Potentials (BOP) which can be employed in real space atomistic calculations. The cohesive energy is composed of the bond energy that contains the covalent character of bonding, an environment dependent central-force term representing the overlap repulsion arising from the valence sp electrons, and a pair potential term representing short-range repulsions. In this paper we present recently constructed BOPs for Ti-Al alloys, originally fitted to reproduce the equilibrium structure and properties of the TiAl with $L1_0$ structure. Only the valence d-electrons are retained explicitly on Ti sites and the p-electrons on Al sites and the orthogonal basis and two-center bond integrals are used. We first discuss the transferability of these integrals which has been thoroughly investigated with the help of ab-initio FP-LMTO calculations. We then present analysis of the stability of the $L1_0$ structure relative to alternative structures, in particular hexagonal B19 and cubic B2, and demonstrate that the same potentials can also be used for Ti_3Al where they favour the hexagonal DO_{19} structure over the cubic $L1_2$ structure. Finally,

results of atomistic studies of stacking-fault type defects, dislocations and twin-like interfaces, encountered in lamellar TiAl, will be presented.
This research was supported in part by the National Science Foundation grant no. DMR99-81023 and U.S. Department of Energy, Basic Energy Sciences through grant no. DE-FG02-98ER45702 (SZ and VV).

2:15 PM Z6.3
BOND-ORDER POTENTIALS WITH ANALYTIC ENVIRON-MENT-DEPENDENT TIGHT-BINDING INTEGRALS: APPLI-CATION TO BCC TRANSITION METALS. Matous Mrovec, Vaclav Vitek, University of Pennsylvania, Dept. of MS&E, Philadelphia, PA; Duc Nguyen-Manh and David Pettifor, University of Oxford, Dept. of Materials, Oxford, UNITED KINGDOM.

We present a new Bond-Order Potential (BOP) for molybdenum in which the environmental dependence of two-centre tight-binding bond integrals has been implemented via a recently developed analytic expression. These bond integrals reproduce very well the numerical ab-intio values of screened LMTO bond integrals. In particular, they display the large discontinuity in ddπ between the first and second nearest neighbour of the bcc lattice whereas they do not show any discontinuity in ddσ. This dependence can be traced directly to the angular character of the analytic screening function and is shown to be critical for the behaviour of the second nearest neighbour force constants. The new BOP eliminates the problem of an unstable T2 phonon mode at the N point that is found in most two-center tight-binding models. Using these potentials we have calculated the γ-surface energies related to dislocation core structures, discussing then the importance of the environment-dependence of the bonding. This work is supported by the U.S. Department of Energy, BES Grant no DE-PG02-98ER45702 and Advanced Strategic Computing Initiative of the U.S. Department of Energy through LLNL, Grant no. B501663.

2:30 PM Z6.4
LATTICE TRAPPING EFFECTS IN Fe USING A POTENTIAL BASED ON EXPERIMENTAL DATA AND AB-INITIO CALCULATIONS. D. Farkas, Department of MS&E, Virginia Polytechnic Institute and State University, Blacksburg, VA; M.J. Mehl and D.A. Papaconstantopoulos, Center for Computational Materials Science, Naval Research Laboratory, Washington, DC.

A recent approach to the development of many-body interatomic potentials for mono-atomic metals with improved accuracy and reliability is tested for the possibility of constructing a more accurate potential for bcc and fcc Fe. The functional form of the potentials is that of the embedded atom method and the database used for the development of a potential includes both experimental data and a set of energies of various metastable alternative crystalline structures of the material generated by ab-initio calculations. The potential accurately reproduces the basic equilibrium properties of Fe including the elastic constants, the phonon properties, the vacancy formation and migration energies. They also predict the correct relative stability of different alternative structures with coordination numbers ranging from 12 to 4. The potentials were used to study lattice trapping effects in the fracture of Fe at low temperature and the results show significant lattice anisotropy, with lattice trapping effects favoring 100 cleavage.

3:15 PM Z6.5
HYBRID QUANTUM MECHANICAL/MOLECULAR DYNAMICS SIMULATION ON PARALLEL COMPUTERS: DENSITY FUNCTIONAL THEORY ON REAL-SPACE MULTIGRIDS. Shuji Ogata, Yamaguchi Univ, Dept of Applied Sciences, Ube, JAPAN; Fuyuki Shimojo, Hiroshima Univ, Faculty of Integrated Arts and Sciences, Higashi-Hiroshima, JAPAN; Aiichiro Nakano, Priya Vashishta, Rajiv K. Kalia, Louisiana State Univ, Dept of Physics and Astronomy, Baton Rouge, LA.

A hybrid quantum mechanical/molecular dynamics simulation scheme is developed, in which a quantum mechanical system described by the density functional theory on real-space multigrids is embedded in a classical system of atoms interacting via an empirical interatomic potential. Handshake atoms coupling the quantum and the classical systems are treated by a novel scaled position method. The scheme is implemented on parallel computers using both task and spatial decompositions. An application to oxidation of Si (100) surface demonstrates seamless coupling of the quantum and the classical systems.

3:30 PM Z6.6
NEW APPLICATIONS OF THE NRL-TB METHOD. M. Mehl, D.A. Papaconstantopoulos, Center for Computational Materials Science, Naval Research Laboratory, Washington, DC; M. Lach-Hab, George Mason University, Fairfax, VA.

The NRL developed tight-binding method (NRL-TB) has been very successful in describing the properties of non-magnetic elemental metals and semiconductors with accuracy comparable to first-principles methods. Using scalable computers we have run molecular dynamics simulations on systems containing hundreds of atoms, and we can calculate forces on systems containing up to two thousand atoms. In this paper we discuss extensions of the method to magnetic systems, specifically the 3d elemental systems, and binary alloys, including Cu-Au and several lead chalcogenides. We first show that the method correctly predicts equilibrium ground state structures, elastic constants, and phonon frequencies. We will then show how the magnetic calculations can be extended to non-collinear systems, and look at the behavior of a domain wall in iron.

3:45 PM Z6.7
PARALLEL TIGHT-BINDING SIMULATIONS OF NANOPHASE CERAMICS: ATOMIC AND ELECTRONIC TRANSPORT AT GRAIN BOUNDARIES. Kenji Tsuruta, Hiroo Totsuji, Chieko Totsuji, Okayama Univ., Dept. of Electrical and Electronic Engineering, Okayama, JAPAN.

Parallel tight-binding molecular dynamics (TBMD) simulations are performed to study structural and electronic evolutions in sintering of nanophase ceramics [1] such as n-SiC and n-TiO_2. We employ an order-N method based on the Fermi-operator expansion method (FOEM) [2]. Sintering simulations of n-SiC show that at elevated temperature process of grain-boundary formation depends strongly on contact angles between two grains. Atomic diffusion in the necks and its effects on the neck growth are evaluated in the TBMD simulations. Also, effects of the mutual grain angles on electron transport at the grain boundary are investigated through a TB representation of the Kubo-Greenwood formula for conductivity [3]. From these analyses, we will discuss a scheme to evaluate the driving force for grain-boundary motions, which will be useful for multiscale simulations of synthesis of nanophase systems.
[1] K. Tsuruta et al., MRS Symp. Proc. vol. 581 (2000), in press.
[2] S. Goedecker, Rev. Mod. Phys. **71**, 1085 (1999).
[3] S. Roche and D. Mayou, Phys. Rev. Lett. **79**, 2518 (1997).

4:00 PM *Z6.8
ATOMISTIC MEASURES OF DEFECT MOBILITY, DOMAIN-SURROUNDING COUPLING, AND MICROSTRUCTURAL DEFORMATION. Wei Cai, Ju Li, Maurice de Koning, Vasily Bulatov, Sidney Yip, Massachusetts Institute of Technology, Dept. of Nuclear Engineering, Cambridge, MA.

We discuss three contributions, each addressing an aspect of micro-meso connection in multiscale simulation, a kinetic Monte Carlo approach linking atomistic simulations of dislocation core energetics to single-dislocation mobility that is directly observable, a linear response theory method to determine the dynamical coupling of a linear elastic medium to an atomistic simulation domain, and a local interaction-based formulation of the thermodynamic driving force for the atomistic analysis of evolving micorstructural defects. Our Monte Carlo study concerns the velocity of a dissociated screw dislocation in Si where kink nucleation, migration, and annhilation processes are treated in terms of activation energies determined by potential model and first-principles calculations. We find a compatibility condition involving the separation between partials and the period of the Peierls barrier, leading to an explanation of an observed stress-threshold behavior which also clarifies the origin of obstacles to kink motion long invoked in the literature. This is an example of temporal coarse-graining, extending the time interval of simulation over molecular dynamics by 7 orders of magnitude. For simulations which adopt a domain decomposition strategy, we show how an atomistic simulation region can be optimally coupled to a linear elastic surrounding. The approach entails the direct systematic evaluation of memory function kernels in the formalism of linear response theory, with minimal elastic wave reflections at the boundary. The resulting time-dependent boundary condition could prove to be useful in coupling molecular dynamics and finite-element simulations. In atomistic simulations of defect mobilities and interactions, the concept of stress field may become inapplicable at the nanometer level, while the concept of energy is still well-defined in the manner of an interatomic potential. 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 J-integral in fracture mechanics. This formulation is applied to a study of dislocation mobility with periodic boundary conditions, in which comparison with linear elasticity results and global free energy calculations will be made.

4:30 PM *Z6.9
MODELING SHOCK-INDUCED PLASTIC FLOW, PHASE TRANSITIONS, AND OTHER CRYSTALLINE CALAMITIES. Brad Lee Holian, Los Alamos National Laboratory, Los Alamos, NM.

Large-scale molecular-dynamics (MD) simulations of shock waves have revealed an amazing degree of complexity in the structures that result from initially perfect crystals. (Pre-existing extended defects introduce even more strange beasts.) At low strengths, uniaxial compression occurs without permanent rearrangement, but with steady waves possible because of elastic distortions transverse to the propagation direction. At a particular critical shock strength in perfect crystals, partial dislocations are emitted at the shock front, for certain crystallographic directions; for others, Martensitic-like transformations occur. Regardless, deformation modes at low shock strength appear to be stress-induced. As shock strength increases, so does the temperature, whereupon a rich variety of deformation modes appear, including thermally activated phase transitions (depending on interatomic interaction potential) and mechanical instabilities. An overview of the zoological diversity of these phenomena will be attempted.

SESSION Z7: POSTER SESSION
MULTISCALE MATERIALS MODELING
Chairs: John L. Bassani and Kyeongjae Cho
Wednesday Evening, November 29, 2000
8:00 PM
Exhibition Hall D (Hynes)

Z7.1
MULTISCALE SIMULATION OF FILM GROWTH AND MICROSTRUCTURE EVOLUTION. David F. Richards[1], Ottmar Klass1, 2, Mark S. Shepherd[2], Timothy S. Cale[1]. [1] Focus Center–New York: Rensselaer, Interconnects for Gigascale Integration, Rensselaer Polytechnic Institute Troy, NY. [2] Scientific Computation Research Center, Rensselaer Polytechnic Institute, Troy, NY.

We present a multiscale method for the simulation of topography and microstructure evolution during thin film growth and processing. Our simulation framework employs a combination of kinetic Monte Carlo techniques for atomic level detail and level set based interface tracking for feature larger scales. Conversion between scales is accomplished using a finite element mesh based "grain-continuum" representations of the film. Meshes can be coarsened to increase the length scale or converted back to atomic scale as needed. The finite element mesh is constrained to conform to nuclei and grain interfaces, and crystal orientation is tracked at all length scales. Grain-continuum representations enable film growth simulations that include nucleation, nuclei growth and coalescence, and feature scale film profile evolution while maintaining microstructural information.

Z7.2
INTEGRATING ATOMISTIC AND CONTINUUM MODELS WITHIN THE DIGITAL MATERIAL SOFTWARE INFRA-STRUCTURE. Chuin-Shan Chen, Cornell Theory Center, Cornell University, Ithaca, NY; Thierry Cretegny, Andrew Dolgert, Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY; Christopher R. Myers, Cornell Theory Center, Cornell University, Ithaca, NY; James P. Sethna, Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY; Anthony R. Ingraffea, Cornell Theory Center, Cornell University, Ithaca, NY.

We are developing a flexible and extensible software infrastructure, Digital Material, to support material modeling at different length scales. We use a mixed atomistic-continuum approach, the quasicontinuum method, to show our novel software techniques at work. We previously developed separate molecular dynamics and finite element codes with an eye for flexibility and efficiency. Because the quasicontinuum method is in some ways a hybrid of the two, it serves as an important test case of our software approach, which emphasizes the use of design patterns to support adaptable software in the solution of new problems. We also show how to use a two-level software architecture, combining low-level numerical kernels written in compiled languages and a high-level interpreted control and integration layer written in the interpreted programming language Python, to provide a powerful environment for material modeling between atomistic and continuum scales. We illustrate our hybrid using examples from intergranular fracture toughness, studying fracture at grain boundaries.

Z7.3
COUPLED ATOMISTIC AND ELASTIC CONTINUUM CALCU-LATIONS USING THE BOUNDARY ELEMENT METHOD. Thomas Lenosky, Babak Sadigh, and Andrew Quong, University of California, Lawrence Livermore National Laboratory, Livermore, CA 94551.

Many problems in materials science are still out of the reach of atomistic methods. Computational methods entail compromises

between the number of atoms that can be treated and accuracy. In many problems of interest, e.g. crack propagation, most of the material can be modeled as an elastic medium with small deformations. In this example only the region near the crack tip must be treated at a atomic level, possibly including electronic structure effects which give rise to chemistry. We have developed a method which allows such an atomistic calculation to be coupled to an anisotropic continuum region, thus letting much larger systems be treated without loss of accuracy. The boundary element method allows the deformations, strains, and stresses in the elastic region to be obtained, given only knowledge of the boundary condition on the surfaces of the medium. Thus it is unnecessary to mesh up the continuum region except for its boundaries. We provide for a smooth matching of the atomistic and continuum regions by embedding additional atoms in the continuum region. Using an empirical potential for silicon as a model system, we have tested our method using cracks under Mode I applied load. We will discuss to what extent the method allows the size of the atomistic region to be reduced, and also discuss possible applications to stress-corrosion cracking.

Z7.4
EXPERIMENTAL ASSESSMENT OF GRADIENT PLASTICITY.
Monica M. Barney, Geoffrey H. Campbell, James S. Stölken, Adam J. Schwartz, Jürgen M. Plitzko, Wayne E. King, Lawrence Livermore National Laboratory, Chemistry and Materials Science Directorate, Livermore, CA; J.W. Morris Jr., Lawrence Berkeley National Laboratory, Materials Sciences Division, Berkeley, CA.

Because classical plasticity models do not take the microstructure into account, they fail to display the length scale effect that is seen experimentally. The mechanics community is actively involved in the development of strain gradient plasticity theories to account for this discrepancy. Two approaches that have recently appeared in the literature are being evaluated. In one approach, originated by N.A. Fleck and J.W. Hutchinson, the strain gradients are considered internal degrees of freedom that require work conjugate higher order stresses. In the other, developed by J.L. Bassani, strain gradients are considered as internal variables that do not introduce work conjugate higher order stresses. Experiments are underway to determine which approach models material behavior accurately with the least amount of complexity. One difference between the two models considered here is the nature of the imposed boundary conditions at material interfaces. Therefore, experiments are carried out using aluminum ultra-high vacuum diffusion bonded between two sapphire crystals loaded under pure shear. Deformed samples are examined with electron backscatter diffraction in the SEM and with various diffraction techniques in the TEM to determine the lattice rotations near the boundary. The experimentally found boundary conditions are subsequently used to determine whether the simpler internal variable model is adequately descriptive or if the greater complexity associated with the internal degree of freedom approach is necessary.

Z7.5
GRAIN FRACTURE MODEL: INFLUENCE OF GRAIN SIZE AND ORIENTATION. Zdenek Knesl, Lubos Nahlik, Institute of Physics of Materials, Dept of Mechanical Properties, Brno, CZECH REPUBLIC; Jan Vrbka, Brno University of Technology, Faculty of Mechanical Engineering, Brno, CZECH REPUBLIC.

Crack propagation in brittle materials is studied as a sequence of breakage of microscopic volume elements, e.g. grains, at the crack tip. According to the linear elastic fracture mechanics the consequent fracture of the grain is postulated to occur when the stress intensity factor at the tip of the crack exceeds the plane strain fracture toughness. In the paper this assumption is modified and a new quantitative model of the grain cracking process is developed and discussed. In the model a grain boundary is taken as an interface between two different materials with their elastic constants depending on the orientation of the grains. Therefore, the behaviour of a crack with its tip at the interface is studied. In this case the stress distribution depends on elastic constants of both materials and, contrary to homogeneous bodies, the stress singularity is of type $r^{-\lambda}$, where the value of the stress singularity exponent λ is in the interval $0 < \lambda < 1$. The stability criterion is then related to the average stress calculated across the distance d from the crack tip, where d is the characteristic dimension of the fractured grain. The value of the average stress $\overline{\sigma}$ is calculated for the maximum value of the normal stress component acting in the grain in front of the crack tip. This value is related to the critical fracture stress σ_{crit}, which is material constant and can be expressed by means of the fracture toughness of the grain. The grain fractured when the average stress $\overline{\sigma}$ exceeds a critical value σ_{crit}. This condition relates the microscopic length parameter d, the orientation of grains, the apparent value of the grain fracture toughness and the macroscopic fracture toughness value. Results contribute to better understanding of the influence of microstructure on bulk properties of materials.

Z7.6
CONNECION OF SLIPPAGE AND RUPTURE OF STRESSED MACROMOLECULAR CHAINS IN DEFORMATION PROCESS OF HIGORIENTED CRYSTALLINE POLYMER. Ulmas Gafurov, Institute of Nuclear Physics, Tashkent, Ulugbek, UZBEKISTAN.

It is suggested the molecular models of chain slippage and rupture of a stressed amorphous section of a passing macromolecule, interrelation of these molecular processes in highoriented loaded amorphous-crystalline polymer. It is taken into account complex interaction between slippage and rupture of polymer chains. An oriented crystalline polymer with homogeneous chemical structure of type of linear polyethylene is examined. The crystalline polymer is considered as two-phasic one with interchanging amorphous and crystalline regions. Using Frenkel-Kontorova's dislocation or soliton models the tension and slippage of macromolecules is considered. It is considered a linear molecular chain rigidly fixed on polymer crystallite surfaces. The activation energy of the slippage and the thermofluctuation rupture of the linear chain is calculated by using Morza's potential for the covalent bond. It is considered conditions under which thermofluctuation rupture of a stressed macromolecular chain takes place. In the course of deformation molecular processes with the changes of local loads, amorphous regions length, conformational structure of passage macromolecules the conditions of the slippage and chain rupture changes consequently.

Z7.7
SELF-AFFINITY ANALYSIS OF THE FRACTURE SURFACES OF POLYPROPYLENE AND OPAL GLASS. M. Hinojosa, C. Guerrero and U. Ortiz, FIME UANL, MS&E Dept, San Nicolas de los Garza, Nuevo Leon, MEXICO.

In this work we report the self-affinity analysis of the fracture surfaces of a polymeric semicrystalline material and an opal glass. In the case of the plastic material, samples of isotactic polypropylene were prepared by varying the cooling rate from the melt; this resulted in different spherulite sizes. Samples were then broken in bend test after being immersed in liquid nitrogen. In the case of the opal glass, samples with different sizes of the opacifying particles, obtained by different thermal treatments, were broken in a punch test. In both cases the fracture surfaces were analyzed by atomic force microscopy (AFM) in the contact mode. Self-affinity analysis was performed by the variable bandwidth method, covering a range of length scales spanning from a few nanometers up to ten micrometers. The roughness exponents are found to be of similar values close to 0.8 with the correlation length corresponding to the size of the spherulites in the plastic material and to the size of the opacifying particles in the opal glass. These results should be taken into account in the development of multiscale models and simulations of the fracture process of real heterogeneous materials.

Z7.8
TRANSITION REGIME FRACTURE TOUGHNESS- TEMP-
ERATURE PROPERTIES AND CONSTITUTIVE BEHAVIOR OF TWO ADVANCED FERRITIC-MARTENSITIC STEELS.
Philippe Spätig, Max Victoria, Centre de Recherches en Physique des Plasmas, Ecole Polytechnique Federale de Lausanne, SWITZER-LAND; George Robert Odette, Glenn Lucas, Eric Donahue, Dept. of Chemical Engineering, University California, Santa Barbara, CA.

Advanced martensitic steels are leading candidate materials for fusion reactor structural components due to their resistance to void swelling, and good balance of physical and mechanical properties. However, irradiations at temperatures below about 400°C result in increases in the cleavage-to-microvoid coalescence transition temperature, as well as reductions in the upper-shelf tearing toughness. This paper reports on the basic constitutive behavior and the transition regime fracture toughness properties of two unirradiated 7-9Cr martensitic alloys, F82H and T91. The constitutive relations presented are based on dislocation mechanics model. Effective fracture toughness-temperature curves, K(T), were measured in the transition regime using relatively small pre-cracked specimens. In many cases the small specimen tests exceed the small scale yielding constraint limits imposed by standard elastic-plastic fracture mechanics. It is shown that the effective toughness can be constraint corrected to small scale yielding limits using FEM simulations of large scale yielding crack tip stress-strain fields combined with micromechanical models of cleavage initiation toughness. Scanning electron microscopy and confocal microscopy fracture reconstruction studies of specimens tested over a range of temperatures were used to characterize the general fracture surfaces and to examine closely key local events that appear to be the primary sources of cleavage. Modest differences in K(T) curves between F82H and T91 appear to be attributable to different athermal component of the yield stress. The temperature shift of K(T) is related to that of the yield stress via the equivalent yield stress model.

Z7.9
THE EFFECT OF LOADING RATE ON THE MECHANISM OF PLASTIC DEFORMATION IN BISMUTH STUDIED BY INSTRUMENTED SHARP INDENTATIONS. <u>Sergey N. Dub</u>, Institute for Superhard Materials, Kiev, UKRAINE; Oleg M. Ostrikov, Pedagogical Institute, Mozyr, BELARUS.

Bismuth is an interesting model material because it is capable of plastic deformation by two micromechanisms (slip and twinning). During microhardness tests with manual load application (loading time being below 1s), both these mechanisms act simultaneously. Slip lines and wedge-like twins are observed around the indent in bismuth in the load range from 100 to 200 mN. To study the mechanism of plastic deformation in more details, the nanohardness tests of bismuth single crystal by Berkovich indenter have been performed. The tests were carried out on (111) plane at loads up to 200 mN and loading rates from 1 to 10 mN/s. Loading rates during nanoindentation were at least an order of magnitude lower as compared to those in microhardness tests. Decrease in the loading rate results in disappearing of twins around the indent in bismuth. Thus, only slip occurs during plastic deformation at a low loading rate. Modeling of the bismuth behavior during indentation shows that one more deformation micromechanism (mechanical twinning) at high loading rates is due to activation of the generation of dislocations.

Z7.10
A THEORY FOR MULTI DAMAGE EVALUATION OF TiN THIN FILM. <u>Kazunori Misawa</u>, Keio University, Department of Mechanical Engineering, Yokohama, JAPAN; Tomonaga Okabe, The University of Tokyo, Graduate School of Frontier Sciences, Tokyo, JAPAN; Masaaki Yanaka, Toppan Printing, Saitama, Japan, Masao Shimizu, Keio University, Department of Mechanical Engineering, Yokohama, JAPAN; Nobuo Takeda, The University of Tokyo, Graduate School of Frontier Sciences, Tokyo, JAPAN.

The present paper proposes a new approach to predict the damage process of TiN thin film under monotonic loading. Elastoplastic shear-lag approach, which considers a nonlinear stress-strain curve of the substrate, has been developed to obtain the stress distribution and to determine the film crack point. In order to assert the validity of the present approach, we conducted the elastoplastic FEM analysis based on the strain incremental theory. The present results have good agreements with FEM results. The strength properties of TiN thin film were obtained with Monte Calro Simulation using the present approach, and favorably compared with experimental results.

Z7.11
MODELLING OF HETEROGENEITIES IN A IF Ti STEEL. Philippe Erieau, <u>Thierry Hoc</u>, Colette Rey, Ecole Centrale Paris, Chatenay Malabry, FRANCE; Herve Biausser, Ecole Centrale Paris, Chatenay Malabry, FRANCE.

In recent years, particular attention has been paid to the anisotropic work-hardening of polycrystalline metals submitted to large strains. Most of the previous studies were devoted to the modelling of cold forming process and to the understanding of the underlying physical mechanisms (e.g. microstructure and texture evolutions). These models based on homogeneisation techniques (Taylor's model, self-consistent scheme) don't take into account the position of each grain in the aggregate, their exact shape and the effect of grain size. In this work, finite element formulation is presented for modelling microstructural evolution and strain heterogeneities evolution during cold deformation of steel. An actual layer of grains (constituted by several grains which orientations are determined experimentally by using the EBSD technique) is used in this simulation. The constitutive law is a viscoplastic power law based on a hardening matrix depending on the dislocation densities on each slip systems. Such a model allows us to represent the anisotropy and the dislocation microstructure evolutions. Moreover, the explicit discretization of grains in finite element technique allows us to compute changes in grain shape and the evolution of strain and lattice rotation fields. A quantitative distribution of stored energy can be then deduced. Different hardening laws are tested in order to determine the influence on the distribution of this stored energy. In order to validate the numerical approach, experiments are performed through channel die testing using microgrids microextensometry to analyse the actual deformation of the polycrystal and to reveal the presence of localization. These results and the texture evolution of the sample are compared with the ones predicted from the simulations.

Z7.12
MODELLING THE EFFECT OF CRYSTALLOGRAPHIC TEXTURE IN PIEZOELECTRIC POLYCRYSTALS. <u>R. Edwin Garcia</u>, W. Craig Carter, Massachusetts Institute of Technology, Dept. of Materials Science and Engineering, Cambridge, MA; Stephen Langer, Edwin R. Fuller, National Institute of Standards and Technology, Gaithersburg, MD.

While the piezoelectric response of a homogeneous phase may be understood through either empirical or first principles calculations. However, the macroscopic response of a polycrystalline piezoelectric material is not amenable to direct analysis because of constraints due to compatibility. In a polycrystal, the state of stress will depend on geometrical effects such as grain size and morphology as well as the degree of crystallographic alignment (texture). Furthermore, the microscopic stress state will also depend on residual stresses from processing and whether microscopic defects develop, either as a result of processing or from subsequent poling. Prediction of macroscopic response requires a model that incorporates all pertinent spatial and crystallographic aspects of microstructure and allows coupling between fields indirectly through coupled single crystal material properties. We examine the role of microstructure in polycrystalline piezoelectric materials by combining finite element techniques with image and orientation data from computer generated microstructures. We demonstrate a technique for predicting microstructural effects on the effective piezoelectric moduli under isothermal conditions by studying the effect of texture and number of grains with a reduced set of microstructural parameters by using the March-Dellose distribution function for a one textured axis. The entire range of Multiples of Random Distribution (MOR) and the effect of number of grain size are analized. We propose scaling relations between the different physical parameters of the system in order to reduce the number of degrees of freedom. We also analyze the role of grain boundaries in determining the macroscopic response of the solid.

Z7.13
Abstract Withdrawn.

Z7.14
SELF-INTERSTITIAL–DISLOCATION INTERACTION AND THE D1 TO D4 OPTICAL BANDS IN PLASTICALLY DEFORMED SILICON. A.T. Blumenau, School of Physics, University of Exeter, Exeter, UNITED KINGDOM and Theoretische Physik, Universität Paderborn, Paderborn, GERMANY; R. Jones, School of Physics, University of Exeter, Exeter, UNITED KINGDOM; S. Oberg, Department of Mathematics, Lulea University of Technology, Lulea, SWEDEN; <u>T. Frauenheim</u>, Theoretische Physik, Universität Paderborn, Paderborn, GERMANY; P.R. Briddon, The University of Newcastle Upon Tyne, Newcastle Upon Tyne, UNITED KINGDOM.

We investigate the interaction of self-interstitial aggregates with the 90° partial dislocation in Si. For our calculations we use the density functional based tight binding method $DFTB$ and the *ab initio* pseudopotential code $AIMPRO$. The latter is very precise concerning the electronic structure and allows the calculation of optical properties. However it is only applicable for rather small systems if used for geometrical optimisation. $DFTB$, however, allows optimisation for cluster sizes up to 2000 atoms on a Cray T3E. Thus, combining both methods, we are able to gain geometrical and energetical information on the scale of several unit cells, as well as precise results on eigenstates localised at only one or two atoms. Applying this concept, we find that I_4 is bound to the dislocation line with an energy of around 3 eV. The defect induces deep levels in the band gap and optical transitions between these levels may account for the D1 to D4 photoluminescent bands relating to plastically deformed Si.

Z7.15
FROM SMALL METAL PARTICLES TO BULK METALS. THEORETICAL APPROACH. <u>Adham Paiziev</u>, Inst. of Electronics, Dept. of Positron Diagnostics, Tashkent, UZBEKISTAN.

For the theoretical analysis of physical processes happening in metal systems of a nanometer scale (metal catalysts, island metal films, ultra disperse metal powders, layer high-temperature superconductors and heterostructures etc.) it is necessary to develop simples theoretical models, capable obviously to explain large number of the experimental facts connected with dimensional effects in metal systems of final sizes beginning from atomic sizes down to massive metals. In the present work the model of a metal system of final sizes is offered. According to this model conductivity electrons are considered closed in spherical (or one dimensional) potential wall limited as sizes of the sample. Within the framework of such model from the first principles the wave functions electrons in metal of final sizes (MFS) and spectrum of energy levels of electrons are defined. For it the Schrodinger equations with boundary conditions on a surface of the limited metal is decided. With the help of offered model the following problems are solved; Account of volt current performances (VCP) of island metal films recordings for Ag island size 10-50A. It shown, that VCP has a S-like character, that will be agreed with experimental data. The passage to the limit to a case of systems of atomic sizes (negative ions, formulae of Demkov-Firsov) and to a case of massive metals (formulae of Fauler -Nordhem) is analyzed. Proceeding from the indicated above representations about MFS a

problem about a behavior of conductivity electrons in a carbon cluster C-60 and carbon nanotubes theoretically is decided.

Z7.16
MICROSCOPIC STRUCTURE OF THE $\Sigma 3$ (112) [1$\bar{1}$0] SYMMETRICAL TILT GRAIN BOUNDARIES IN NIOBIUM AND MOLYBDENUM. T. Ochs, C. Elsässer, H. Haas, Max-Planck-Institut für Metallforschung, Stuttgart, GERMANY.

The accurate description of interatomic interactions is an important basis for realistic and material-specific theoretical simulations of extended defects like surfaces, interfaces or dislocations. This issue is addressed in the present work for the case of grain boundaries in metals.
The $\Sigma 3$ (112) [1$\bar{1}$0] symmetrical tilt grain boundary is a twin boundary, which is frequently formed during plastic deformation of body-centered cubic transition metals. In this work, microscopic translation states and atomistic structures of such boundaries in Niobium and Molybdenum were investigated by means of two total-energy approaches: a first-principles mixed-basis pseudopotential method, which is based on the local density functional theory, and a semi-empirical environment-dependent spd-basis tight-binding model. Both schemes accurately account for distance- and angle-dependencies of interatomic interactions via the explicit treatment of the electronic structure in the calculation of total energies and forces.
As results of both theoretical approaches for Mo, two metastable interface structures were obtained, one with mirror symmetry and a sheared one, which has a twofold screw-rotation axis along the [11$\bar{1}$] direction. The latter one is found to be energetically preferred by both approaches. The importance of angle-dependent interatomic interactions is illustrated by comparison with other theoretical results obtained for the same boundary in Mo [1], employing empirical interatomic potentials with or without angle-dependent contributions. Experimentally, in a high-resolution transmission-electron-microscopy study two different microscopic grain-boundary structures were observed. This study, however, was not decisive about their energetics.
[1] A.G. Marinopoulos et al., Phil. Mag. A **72** (1995) 1311.
[2] S. Tsurekawa et al., Mater. Sci. Eng. A **176** (1994) 341.

Z7.17
Al GRAIN BOUNDARY EMBRITTLEMENT PROMOTED BY Na IMPURITY: AN AB INITIO STUDY. Guang-Hong Lu, Ryoichi Yamamoto, Inst of Industrial Science, Univ of Tokyo, Tokyo, JAPAN; Masanori Kohyama, Dept of Materials Physics, Osaka National Research Inst, AIST, Osaka, JAPAN.

It has been reported[1] that Na as impurity in Al-Mg alloy tends to segregate in Al grain boundaries and thus induces embrittlement. We therefore choose Na as impurity and Al as host metal to present ab initio pseudopotential calculation bases on density functional theory (DFT) and local density approximation (LDA). We construct an 84-atom model with Al $\Sigma 9$[110] tilt grain boundary, in which 4 atoms are substituted by Na impurity atoms. The pseudopotential of Al is constructed based on TM scheme[2], and that of Na is constructed based on HSC scheme[3] with partial core correction. We calculate the stress using Nielsen-Martin scheme[4]. Relaxed construction, valence charge density and local density of states (LDOS) of Al grain boundary with and without Na impurity atoms were calculated, respectively. The results shows that by Na segregation the grain boundary expands, the charge density around the Na atoms and along the boundary decreases significantly. The significant decrease of the valence charge density in the Al grain boundary means the formation of the weak bond regions. As compared with the pure boundary, there exist several weak Na-Al bonds and weak Al-Al bonds at the boundary with the segregated impurities. Such weak bond region should act as the origins of the crack or the preferential path of the cracks. Furthermore, ab initio tensile test was applied on the same model, and the stress-strain relations has been obtained.
[1] H. Okada, M. Kanno, Scripta Materialia 37, 781 (1997).
[2] N. Troullier and J.L. Martins, Phys. Rev. B 43, 1993(1991).
[3] D.R. Hamann, M. Schlüter and C. Chiang, Phys. Rev. Lett. 43, 1494(1979).
[4] O.H. Nielsen, R.M. Martin, Phys. Rev. B, 32, 3780(1985).

Z7.18
FROM MOLECULAR TO CONTINUUM MECHANICS BY PROBABILISTIC APPROXIMATION: THE CRUCIAL ROLE OF BOUNDARY CONSTRAINTS. Yitzhak Shnidman, Polytechnic Univ, Dept of Chemical Engr and Chem, Brooklyn, NY.

Molecular dynamics (MD) simulations provide a realistic description of nanostructural time evolution in molecular systems, but the fastest motions typically limit the timestep to the femtoseconds range. This severely constrains the number of particles in a simulation, may preclude simulation of long relaxation times needed to overcome trapping in local minima, and thus degrades the quality of trajectory

averages needed to make the connection to continuum mechanics and rheology.
We will show how to overcome these limitations by a self-consistent probabilistic approximation of Newtonian evolution of coordinates and momenta. If the system is unbounded, this goal is achieved by closed time evolution of their first and second moments with respect to a Gaussian approximation of single-particle probability distributions and potentials. This allows us an explicit connection to continuum mechanics and rheology, relating local mass and momentum conservation laws to convective and diffusive currents depending explicitly on molecular potentials and couplings to external reservoirs. However, MD simulations of condensed systems typically require confining a finite number of molecules to a volume with periodic boundary conditions. This implies that both particle probabilities and potentials are periodic functions, for which a Gaussian approximation is inappropriate. We will show that for such systems, efficient probabilistic evolution equations can be derived for a closed set of amplitudes in a truncated Fourier decomposition of effective singlet probabilities and potentials. These equations will be related to continuum mechanics and rheology in Fourier space.

Z7.19
NEW ALGORITHM FOR INCREASING TYPICAL TIME STEPS IN MOLECULAR DYNAMICS SIMULATON. Z.M. Khakimov, Inst of Nuclear Physics of Uzbek Acad of Sciences, Tashkent, UZBEKISTAN.

In the molecular dynamics (MD) simulation of various phenomena in solids there is a great demand for algorithms allowing to employ a long time step dt in the integration of equations of motion, satisfying at the same time the energy conservation (EC) law with acceptable accuracy. In this report we present new algorithm based on the using of first derivatives of accelators, $b(x)$, with respect to particle coordinates x at a current time t. The cost paid for calculation of these derivatives is not essential as compared with savings of computational time provided by the algorithm that can increase dt by one order of magnitude at least for typical MD simulations. Equations for particle's coordinates x and velocities v are (a is particle's acceleration)

$$x(t+dt) = x(t) + \frac{\left\{ v(t)dt + \frac{[7a(t)-a(t-dt)]dt^2}{12} \right\}}{\left[\frac{1-b(x)dt^2}{12} \right]}$$

$$v(t+dt) = v(t) + \frac{[8a(t)+5a(t+dt)-a(t-dt)]dt}{12}$$

This algorithm uses one more word of storage than popular velocity Verlet algorithm (VVA), but unlike Beeman algorithm that also uses this extra word of storage, leads to dramatic improvement in satisfaction of EC-law as compared with VVA. For instance, for particles moving in the harmonic potential well this improvement is about five orders of magnitude at dt=0.0001 and two orders of magnitude at dt=0.1, while Beeman algorithm improves EC only three times in these time limits. Detailed comparison of this algorithm with existing ones will be provided for photoinduced defect dynamics in silicon clusters using self-consistent tight-binding molecular dynamics approach.

Z7.20
LONG SCALE MONTE-CARLO SIMULATION OF GRAIN GROWTH AND GRAIN BOUNDARY SEGREGATION IN BINARY ALLOYS. J.-M. Liu, Z.G. Liu, Nanjing University, Laboratory of Solid State Microstructures, Nanjing, CHINA.

Grain growth and grain boundary segregation in binary alloys as concurrent sequences over long time scale are simulated using a kinetic Monte-Carlo algorithm based on Q-state Potts model. First, the static property of the hybrid system is studied, predicting a weak effect of grain growth and grain boundary segregation on the critical point of the phase precipitation. Very different kinetic behaviors of the hybrid system over early stage and late stage have been identified with a detailed analysis of the kinetics of grain growth and phase precipitation.

Z7.21
HIGH TEMPERATURE THERMAL CONDUCTIVITY OF CRYSTALLINE AND AMORPHOUS SiO_2 BY THE EQUILIBRIUM MOLECULAR DYNAMICS. Hideo Kaburaki, Hajime Kimizuka, Center for Promotion of Computational Science and Engineering, Japan Atomic Energy Research Institute, Tokyo, JAPAN; Ju Li, Sidney Yip, MIT, Dept of Nuclear Engineering, Cambridge, MA.

Thermal conductivity of amorphous SiO_2 shows a large reduction compared to crystalline state and its temperature dependence exhibits an intrinsic property common to all amorphous solids. The basic understanding of this property is still lacking. We focus on the molecular dynamics study on the high temperature thermal conductivity of crystalline (α-quartz) and amorphous SiO_2 above

approximately 30K. Thermal conductivity of crystalline state varies as typically T^{-1} while that of amorphous state tends to increase. The standard theory of phonon Boltzmann equation with the relaxation time approximation applies to the crystalline state but is known to fail for the amorphous state. We try to take another look at both of these states and apply the equilibrium molecular dynamics method using the Green-Kubo formula. This approach has been verified to reproduce well the absolute values and the temperature dependence of thermal conductivity for the solid argon crystal if the appropriate interatomic potential is used. We used the BKS (van Beest-Krammer-van Santen) potential, which is known to exhibit the elastic constants properly, and apply it to calculate the thermal conductivity of crystalline and amorphous state with the number of 2268 particles. We obtained the temperature dependence of thermal conductivity that can be compared with experiments. The results of the autocorrelation function of heat flux are shown to exhibit a new look at the mechanism of thermal conduction.

Z7.22
PARTICLE-MESH-EWALD APPROACH TO FIXED AND INDUCED MULTIPOLAR INTERACTIONS. Celeste Sagui, Laboratory of Structural Biology, National Institute of Environmental Health Sciences (NIEHS), Research Triangle Park, NC; Abdulnour Toukmaji, John Board, Department of Electrical Engineering, Duke University, Durham, NC; Tom Darden, Laboratory of Structural Biology, NIEHS, Research Triangle Park, NC.

Despite the enormous increases in computer power and algorithmic advances, the accurate simulation of biologically active macromolecules remains a formidable challenge. In particular, the representation and computation of long-range electrostatic interactions is a bottleneck for classical potential-based simulations. In these simulations, the charge density of atoms, is assumed to be fixed independently of other atoms. Most current macromolecular force fields do not include terms to model induction or charge transfer, which describe the rearrangement of electron density as a function of the local electric field. The correct and efficient treatment of higher order multipoles and polarization constitutes an important bridging step between classical and quantum descriptions. Although there exist several approaches to incorporate induction effects in classical macromolecular force fields, they are generally too costly for widespread use. We have recently expanded the Particle-Mesh Ewald (PME) method to treat point charges and fixed or induced dipoles [1]. During MD the induced dipoles can be propagated along with the atomic positions either by iteration to self-consistency at each time step, or by a Car-Parrinello (CP) technique using an extended Lagrangian formalism. We present the derivation of the new algorithm and a study of its accuracy, efficiency and effect on calculated properties of a polarizable water model. The use of PME for electrostatics of fixed charges and induced dipoles together with a CP treatment of dipole propagation in MD simulations leads to a cost overhead of only 33% above that of MD simulations using standard PME with fixed charges, allowing the study of polarizability in large macromolecular systems. The generalization to multipoles of arbitrary order will be also discussed.
[1] A. Toukmaji, C. Sagui, J. Board, and T. Darden, J. Chem. Phys. (2000).

SESSION Z8: POLYCRYSTALLINE PLASTICITY –
GRAIN SIZE AND DISTRIBUTION EFFECTS
Chairs: Diana Farkas and Darcy A. Hughes
Thursday Morning, November 30, 2000
Independence W (Sheraton)

8:30 AM *Z8.1
TAYLOR-BASED NONLOCAL THEORY OF PLASTICITY.
Y. Huang, Univ of Illinois, Dept of Mechanical Engineering, Urbana, IL; H. Gao, Stanford University, Div of Mechanics and Computation, Palo Alto, CA.

A Taylor-based nonlocal theory (TNT) of plasticity is proposed to account for the size dependence of plastic deformation at micron and submicron length scales. This theory is intended to link Taylor's model of dislocation hardening to a nonlocal theory of plasticity in which the density of geometrically necessary dislocations is expressed as a nonlocal integral of the strain field. It connects the plastic deformation at the micron scale to the Taylor model in dislocation mechanics via a multiscale, hierarchical framework. The theory does not involve higher-order stresses, does not require additional boundary conditions as compared with the classical theories of plasticity, and therefore preserves the structure of classical plasticity. Numerical methods have been developed for TNT plasticity. We show that the predictions of TNT plasticity agree very well with the micro-indentation hardness experiments, as well as with micro-torsion and micro-bending experiments.

9:00 AM *Z8.2
COSSERAT MODELING OF SIZE EFFECTS IN THE MECHANICAL BEHAVIOUR OF POLYCRYSTALS AND MULTIPHASE MATERIAL. Samuel Forest, Ecole des Mines de Paris-CNRS Centre des Materiaux, Evry, FRANCE.

Classical homogenization techniques are not designed to predict the effect of the size of the constituents on the effective mechanical behaviour of heterogeneous materials. They usually take the volume fraction and, in some cases, the morphology of phase distribution into account. This shortcoming is related to the fact that, in crystals, the elastoviscoplastic behaviour of each constituent within the aggregate may be different from that observed on the constituent alone (say the single crystal). Cosserat single crystal plasticity is used in this work to describe the influence of grain size on the effective non-linear behaviour of polycrystals. For that purpose, three-dimensional finite element calculations of random or periodic Cosserat multi-crystalline aggregates of different grain sizes are provided. The polycrystal is regarded as a heterogeneous Cosserat medium and specific techniques for the estimation of the effective properties are presented. The approach is then applied to the case of two-phase single crystal materials for which the behaviour of one phase as a matrix turns out to be strongly harder than the isolated phase.

9:30 AM Z8.3
PRIMARY CREEP IN POLYCRYSTALLINE ALPHA TITANIUM: COUPLED OBSERVATIONS AND A STOCHASTIC CELLULAR AUTOMATON MODEL. Neeraj Thirumalai, Michael J. Mills and Glenn S. Daehn, Dept of MS&E, The Ohio State University, Columbus, OH.

The room temperature creep of titanium is rather remarkable. At stresses near the 0.2% yield stress extensive deformation can be observed that is often well approximated by a power law relationship between strain and time at moderate strains. Eventually at rather high strains a linear relation between strain and time sometimes observed. Strains obtained in this mode of deformation can reach several percent at stresses near the yield stress. This remarkable time dependence is largely due to the near-absence of traditional strain hardening mechanisms. This behavior is well modeled by a model that considers a number of different obstacles that are coupled by load shedding. This concept is carried out in a stochastic cellular automaton model that captures many of the features of the experimentally observed in the plastic deformation of weakly-hardening alloys. In the present work the model is shown to be useful in deconvoluting strain-time curves captured at varied stresses and temperatures to reveal the force and temperature dependence of slip of the obstacle population in the microstructure.

9:45 AM Z8.4
FINITE ELEMENT SIMULATION OF A 1000 GRAIN "VIRTUAL TEST SAMPLE". James S. Stölken, Material Science and Technology Division, Lawrence Livermore National Laboratory, Livermore, CA.

The development of physics-based constitutive models of polycrystalline metals under extreme conditions of deformation depends critically upon the proper homogenization of single crystal response. This work aims to provide a "virtual" test-bed on which a variety of single crystal constitutive behavior, grain configurations, and crystallographic textures can be input and the resulting polycrystalline response computed under a broad range of deformation conditions. The computed response may be directly compared with experiments by utilizing as initial input high resolution, three dimensional microstructural data gathered over a large representative volume of material. For the case considered here, a polycrystalline tantalum plate of approximately 30 micron grain size was characterized using a combination of EBSD microscopy and serial section reconstruction. The volume characterized, which is comprised of over 1000 individual grains, consists of approximately $330\Sigma10^{6}$ cubic microns sampled at $\sim$5 micron intervals. This microstructural data was then used as input to a finite element simulation using a crystal plasticity constitutive model. Comparisons of deformation response at varying levels of mesh refinement were used to explore the scaling of simple homogenization methods, such as the Taylor approximation, over a wide range of scales. Comparisons of texture evolution in both the real sample and the "Virtual" test sample may then be compared as a means for polycrystalline model validation. This work is performed under the auspices of U.S. Department of Energy and Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

10:30 AM *Z8.5
INTRINSIC AND EXTRINSIC SIZE EFFECTS IN PLASTICITY.
J. Gil Sevillano, CEIT (Centro de Estudios e Investigaciones Técnicas de Guípúzcoa) and Faculty of Engineering, University of Navarra, San Sebastin, SPAIN.

A classification of size effects (SE) in plasticity is attempted. Any structural size dependent process or property, plasticity for instance, is a manifestation of a size effect. "Intrinsic" SE are perceived when any internal length scale directly influencing some process or property interferes with the size of the material region where the process is going on or when two internal length scales directly affecting the same process or property interfere. "Extrinsic" SE arise from the external imposition of spatial gradients in the process or by the building up of internal gradients by the (externally induced) process itself. In dislocation-mediated plasticity plastic strain gradients are resolved by the storage of geometrically necessary dislocations (GND) leading to prominent size effects. Of course, mixed effects with intrinsic and extrinsic contributions can be found as well as superposed effects involving more than two characteristic lengths (i.e., size effects on size effects). The different action of the two classes of SE on the constitutive equation for plasticity by dislocation glide is signalled. Finally, some technically relevant but up to now overlooked SE examples are presented.

11:00 AM Z8.6
MULTISCALE SIMULATIONS OF GRAIN GROWTH WITH ANISOTROPIC GRAIN-BOUNDARY PROPERTIES AND GRAIN ROTATION. Dorel Moldovan, Dieter Wolf, Simon R. Phillpot and Andrew J. Haslam, Matls Sci Div, Argonne Natl Lab, Argonne, IL.

Building on insights gained from our molecular-dynamics simulations of grain growth we present mesoscopic simulations which fully incorporate the interplay between grain-boundary-migration and grain-rotation driven grain growth; in the latter two neighboring grains coalesce to become one by eliminating their common boundary. By contrast, the conventional picture is that grain growth results solely from the migration of grain boundaries in response to the driving force associated with the reduction in the grain-boundary area. However, our molecular-dynamics simulations suggest that, at least in a nanocrystalline microstructure, grain rotations play an equally important role. Based on this insight we have developed a kinetic model for grain-boundary-diffusion accommodated grain rotation, extending the formalism of Raj and Ashby (1971) for grain-boundary sliding. We have incorporated this model into a mesoscopic-simulation code based on the Needleman-Rice (1980) variational formalism for the dissipated power. The topological, structural and kinetic consequences of including the grain-rotation mechanism in addition to grain-boundary migration are analyzed; in particular, we find that the usual parabolic growth law is modified. Work supported by U.S. Department of Energy, Office of Science, under Contract W-31-109-Eng-38.

11:15 AM Z8.7
FROM PRIMARY DISPLACEMENTS TO FRACTURE TOUGHNESS: PROGRESS ON DEVELOPING AN INTEGRATED MULTISCALE-MULTIPHYSICS MODEL OF IRRADIATION EMBRITTLEMENT. G. Robert Odette, Univ of California, Santa Barbara, CA, Dept of Mechanical & Environmental Engr, Brian D. Wirth, Lawrence Livermore Natl Lab, Chemistry & Matls Sci Div, Livermore, CA and Roger E. Stoller, Metals & Ceramics Division, Oak Ridge National Lab, Oak Ridge, TN.

An integrated multiscale model for irradiation embrittlement of pressure vessel steels is described. The model directly links the following elements: a) energy dependent cross sections for primary defect production based on nuclear data and recoil kinematics codes and molecular dynamics simulations; b) short-to-long time evolution of cascade damage that is correlated in space and time to provides the source term for both freely diffusing defects, as well as small cluster-complexes of defects and solutes, based on kinetic Monte Carlo methods; c) long-range coupled radiation enhanced diffusion of defects and copper leading to annihilation, additional clustering and cluster growth, using rate theory models; d) flows of other alloy solutes to and from precipitates using thermodynamic models; e) hardening by the evolving cluster complexes and precipitates, using Russell-Brown and strength superposition models; f) the relation between fracture toughness and Charpy energy-temperature curves using micro-macromechanical models of cleavage initiation. The input to the model is the alloy composition and microstructure, initial strength and fracture properties as well as the irradiation temperature and neutron flux, spectrum and fluence. The outputs are shifts in both toughness master curve and Charpy indexed transition temperatures. Some components of the model are semiempirical, while others are treated with various level of approximation. In both cases, the integrated embrittlement model can be improved by more rigorous physical treatments of these subprocesses. The model predictions are compared to a large database on the individual and combined effects of metallurgical and irradiation variables. While quantitatively predictive and useful in its own right, the integrated model framework provides a basis for identifying focussed targets for further experiments and models.

11:30 AM Z8.8
MICROMECHANICAL MODELING OF TWO-PHASE STEELS. Mikael Nygards, Department of Solid Mechanics; Dilip Chandrasekaran, Department of MS&E; Peter Gudmundson, Department of Solid Mechanics, Royal Institute of Technology, Stockholm, SWEDEN.

A two-dimensional micromechanical model based on the finite element method is presented to model a two-phase ferrite/pearlite steel, by aid of generalized plane strain elements. A periodic representative cell containing 50 ferrite grains, and the desired fraction pearlite is used. By applying periodic boundary conditions, loading by an average stress or strain state is possible. Uniaxial tensile tests were performed on specimens containing the ferrite and pearlite microstructures, and on two-phase materials containing 25% and 58% pearlite. The stress-strain data of the ferrite and pearlite materials are used to fit Taylor's relation to represent the ferrite and the pearlite workhardening properties. The ferrite model is grain size dependent, while the pearlite model depends on the lamellar spacing. Thereafter, the grain size and the lamellar spacing in two-phase materials are measured, and the total stress-strain response of the materials are modeled. Comparisons between generated data and experiments show good agreement up to a strain of 2%. Moreover, the model is used to investigate the effect of different tensile loading directions as well as pure shear. Results show that the softer ferrite phase is more dominating when loading in the x-, y-direction or by shear. While loading in the z-direction falls very close to the rule of mixture for stresses.

SESSION Z9: POINT DEFECTS
Chairs: Noam Bernstein and David G. Pettifor
Thursday Afternoon, November 30, 2000
Independence W (Sheraton)

1:30 PM *Z9.1
MULTISCALE SIMULATIONS OF DEFORMATIONS OF SOLIDS UNDER EXTERNAL LOADING. Efthimios Kaxiras, Harvard Univ, Dept of Physics and Div of Engineering and Applied Sciences, Cambridge, MA.

Large deformations of solids under external loading defy a simple description based on constitutive laws due to possible phase transformations and the presence of strain way beyond the elastic limit. Chemical reactions in the high-stress environment near a loaded crack tip present an additional complication to the response of the solid and are related to phenomena like corrosion and embrittlement. In these cases, a quantum mechanical approach for simulating electronic behavior is indispensable, as chemical bonds are being broken or rearranged under unusual conditions. However, not all the bonds in an inhomogeneously strained system are subjected to the same amount of distortion; in regions where the distortion of chemical bonds from their equilibrium is small, empirical methods, which are also computationally more efficient, suffice. Combining methodologies that can describe with adequate accuracy the different regions in solids is a challenge to computational modelling. We will discuss recent advances in developing such methodologies and their applications to realistic systems. The applications include intentation of silicon, a prototypical brittle material, the switching mechanism in a pieozoelectric as a function of strain and external electric field, and the simulation of crack behavior in metals in a chemically active environment under external load.
In collaboration with N. Choly, I. Park, G. Smith, E. Tadmor, U. Waghmare, D. Orlikowski, O. Politano.
Work supported by AFOSR/MURI and the Harvard MRSEC funded by NSF.

2:00 PM *Z9.2
MODELLING ELECTROMIGRATION-INDUCED MASS TRANSPORT IN ALLOYS. P. Gumbsch, J.P. Dekker, C. Schmidt, C.A. Volkert, Max-Planck-Institut für Metallforschung, Stuttgart, GERMANY.

Electromigration is atomic transport induced by an electric current. A detailed microscopic understanding of electromigration processes in alloys is still lacking, despite its great technological importance as a failure process in electronic conductor lines. It is, for example, well known that the electromigration performance of aluminium-based alloys is enhanced by the addition of copper and as a result is routinely incorporated in microelectronic interconnects. However, it is still not clear where the effect comes from. To gain some fundamental understanding of diffusion in dilute substitutional alloys under electromigration conditions, we have combined several modelling techniques on different scales in length and time. Firstly, the electromigration wind force on aluminium host atoms and on impurity

atoms is calculated using a Green's function method for the calculation of the electronic structure. It is found that the wind force on aluminium atoms and impurities is quite different and that the wind force on aluminium is changed considerably by the presence of an impurity atom. The results of these calculations are then used as the driving forces in a kinetic Monte Carlo simulation of diffusive transport. For some simple cases, the results of the kinetic Monte Carlo simulations can also be reproduced by an analytical model which is an extension of the five-frequency model, developed for the description of diffusion via the single-vacancy mechanism in dilute alloys. The resulting flux equations shown that the addition of a few atomic percent of alloying atoms can reverse the direction of the flux of host atoms under certain conditions. The flux reversal can slow down electromigration mass transport considerably and explain many of the experimentally observed details of the role of copper in aluminium conductor lines. Also the temperature-dependence is strongly non-Arrhenian and therefore makes extrapolation from test to use conditions non-trivial.

2:30 PM Z9.3
COUPLING-OF-LENGTH SCALES APPROACH FOR SIMULATIONS OF ELECTRONIC DEVICES. Elefterios Lidorikis, Martina E. Bachlechner, Rajiv K. Kalia, Aiichiro Nakano, Priya Vashishta, Concurrent Computing Laboratory for Materials Simulations, Louisiana State University, Baton Rouge, LA; George Z. Voyiadjis, Department of Civil and Environmental Engineering, Louisiana State University, Baton Rouge, LA; Anupam Madhukar, University of Southern California, Los Angeles, CA.

The interface structure and stress distribution in Silicon(111)/a-Silicon nitride nanopixels are studied using molecular dynamics (MD) simulations on parallel computers. Bulk silicon is described by the Stillinger-Weber potential and silicon nitride is presented by a combination of two- and three-body interactions that include steric, charge transfer, polarizability, and covalent forces. Charge transfer at the interface is extracted from self-consistent LCAO electronic structure calculations. The MD simulation for these nanopixels involve different pixel sizes with systems consisting of up to 27 million atoms. In all these systems we find stress domains at the interface which persist into the silicon substrate. The nature of the stress domains will be discussed.
We have also developed a scheme in which the physical system is divided into finite element (FE), MD, and handshake (HS) regions. The HS and FE regions are far away from the process zones. Within the MD region, the dynamics of atoms is governed by suitable potentials as described above, while in the FE region the equations for continuum elastic dynamics are solved on a computational grid. To ensure a smooth transition, the dynamics obeyed by hybrid atoms/nodes in the HS region are governed by the average Hamiltonian of the MD and FE schemes. Future applications will be discussed.

2:45 PM Z9.4
STUDY OF GRAIN BOUNDARY PROCESSES IN ALUMINUM USING THE QUASICONTINUUM APPROACH. L. Gil Espert, Polytechnical University of Catalonia, Barcelona, SPAIN; M.J. Caturla, V. Bulatov, T. Diaz de la Rubia, Lawrence Livermore National Laboratory, Livermore, CA.

Understanding the underlying processes occurring at the grain boundaries of a nanocrystalline material as a function of grain size is necessary in order to explain the mechanical properties of these materials. In the last few years there has been a great success in explaining these phenomena through the use of computer simulations, such as molecular dynamics. However, the size of the grains that can be studied with these methods is limited due to the computational demand of these simulations. Most of the interesting phenomena in nanocrystalline materials happen or are initiated at the grain boundaries, while the center of the grain remains mostly as a perfect crystal structure. In the last few years a powerful model has been developed by Tadmor, Ortiz and Phillips [1] that allows for an adaptive mesh in a molecular static calculation called the quasicontinuum method. This method seems the most appropriate to study grain boundary processes. We have developed a 3 dimensional quasicontinuum code following the model of Tadmor, Ortiz and Phillips. This code has been used to study grain boundary processes in Aluminum, such as grain boundary sliding as a function of an applied load. The results are compared to full atomistic simulations. [1] E.B. Tadmor, M. Ortiz, R. Phillips, Phil. Mag. A (96) 73, 1529. 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.

3:30 PM Z9.5
BEHAVIOR OF GRAIN BOUNDARY RESISTIVITY IN METALS PREDICTED BY A TWO DIMENSIONAL MODEL. Rand Dannenberg, AFG Development Corporation, Petaluma, CA,

Alexander H. King, School of Materials Engineering, Purdue University, West Lafayette, IN.

The behavior of a model for the specific grain boundary resistivity in metallic bamboo conductor lines is developed and compared to other theoretical treatments, and to experiment. The grain boundary is modeled as an array of scatterers on a plane. The scatterers are called vacancy-ion complexes, in which the vacancy represents the boundary free volume, and the ion is an atom adjacent to the vacancy. Three cases are investigated, that of non-interfering scatterers, a continuum of interfering scatterers, and discrete interfering scatterers. The approximations used lead to a specific grain boundary resistivity of the experimentally observed order of magnitude for aluminum, for the first two cases. In the non-interfering case, the specific resistivity is independent of the grain boundary area. For the continuum interfering case it is found that the grain boundary resistivity is only weakly dependent on the grain boundary area, and, that the grain boundary has a high probability of perfect reflection or transmission of incident electrons. The source of resistivity is from reflection of electrons. This behavior is independent of the exact interaction potential between the incident electrons and the defects which comprise the grain boundary free volume. The discrete interfering case produces specific resistivities several of orders of magnitude too large, and a strong dependence on the grain boundary area. A connection is established between the grain boundary resistivity and the electromigration wind force.

3:45 PM Z9.6
ATOMICALLY-BASED FIELD FORMULATIONS FOR COUPLED PROBLEMS OF COMPOSITION AND MECHANICS. Krishna Garikipati, Univ of Michigan, Dept of Mech Engr, Ann Arbor, MI.

Composition occupies a central position in the modelling of semiconductor and microelectronic materials. Examples include the (i) transport of oxygen molecules during thermal oxidation of silicon, (ii) dopant diffusion in silicon, (iii) self-diffusion of metal atoms in interconnect lines and (iv) precipitation of separate phases in patterned structures. In each of these cases, composition and mechanics are, in fact, closely coupled. Thermal oxidation of silicon requires diffusion of O_2 through SiO_2—a process which is depressed or enhanced as the local hydrostatic stress is compressive or tensile. A similar effect is observed in dopant diffusion through silicon. Stress-mediated self-diffusion of metal atoms in interconnect lines is well-established, as is the influence of mechanics upon the energetics underlying phase precipitation. Models for the coupled description of composition and mechanics exist to a lesser (thermal oxidation and dopant diffusion) or greater extent (metal self-diffusion and phase precipitation). *However, a bidirectionally coupled field formulation, accounting for vacancy and interstitially-mediated exchange mechanisms and the associated stress/strain, is not yet in place.* Such a formulation would enable one to pose general, coupled, initial and boundary-value problems. This would eliminate the need to make simplifying assumptions such as regularly shaped domains and known, constant external stress states. Recent results in applying such an approach to the coupling of mechanics and self-diffusion of metal atoms will be discussed (including numerical examples). An extension of these methods to thermal oxidation, dopant diffusion and phase precipitation will be sketched. The approach consists of building appropriate internal energy, external work done and entropy density terms reflecting the atomic-level exchange mechanisms and associated mechanics. *Formal thermodynamic arguments then lead to constitutive field relations reflecting the atomic-level coupling—the multiscale aspect of this approach.* Balance laws, initial and boundary conditions complete the multiscale, coupled field description.

4:00 PM Z9.7
FIRST-PRINCIPLES STUDY OF BORON CLUSTERING IN SILICON. Xiang-Yang Liu[1], Wolfgang Windl[2] and Michael P. Masquelier[1], Computational Materials Group, Motorola Inc. [1]Los Alamos, NM. [2]Austin, TX.

Ion implantation is currently the method of choice to introduce dopants such as B in Si. Thermal anneals are used to heal the implant damage as well as to activate the dopant electrically. The implant-anneal cycle causes transient enhanced diffusion (TED) of B and clustering of B atoms at concentrations far below the solubility limit. The formation of these small immobile B-interstitial clusters (BICs) causes the deactivation of B. In this work, we use density-functional theory calculations to study the B clustering process in Si. We determine the minimum-energy structures of these clusters embedded in Si bulk with different sizes and calculate the energy state of each cluster. Special care is taken with regard to structure minimization, charge state effects and corrections. The energetics of BICs, along with a recently discovered B diffusion mechanism, are implemented into a continuum PDE solver to model the formation, growth, and dissolution of BICs and the TED of B in Si. The predictions are compared with recent experimental annealing activation studies and other experimental data where available.

4:15 PM Z9.8
FEATURES OF VACANCY INTERACTION WITH INTERSTITIAL CLUSTERS IN BCC METALS. M. Pelfort, A. Serra, Dept. Matematica Aplicada III, Escuela de Camins, UPC, Barcelona, SPAIN; Yu.N. Osetsky, MS&E, Dept. of Eng., The University of Liverpool, UNITED KINGDOM.

Recent theoretical calculations and atomistic computer simulations have shown that one-dimensionally (1D) glissile clusters of self-interstitial atoms (SIAs) play an important role in the evolution of microstructure in metals and alloys under cascade damage conditions. Theoretical treatments based on the production bias model (PBM) and cascade-induced source hardening (CISH), clarify many features of materials behaviour by considering 1D glissile SIA clusters. However, further progress in understanding irradiation phenomena demands a detailed knowledge of different reactions where glissile SIA clusters take part. Thus, the latest version of the PBM has demonstrated that there is a significant lack of knowledge of mechanisms such as interaction between mobile clusters and other microstructure components, changes glide directions and reduction of cluster mobility. Some aspects of interactions have been studied recently and formation of immobile complexes of glissile clusters in the bulk and near dislocations has been demonstrated. However, in addition interaction of clusters with each other and with dislocations, their interactions with point defects has to be considered more carefully. Here we present the first results related to interaction between an SIA cluster and vacancy in bcc-iron. The interactions were studied by atomistic simulations and elasticity theory. Some qualitative differences between the results obtained by these two methods were found, thereby demonstrating the need for the atomistic approach. It is shown that interaction with vacancies can reduce and, in some cases, suppress mobility of SIA clusters. The results are discussed in the light of experimental data and theoretical predictions.

4:30 PM Z9.9
ATOMISTIC AND ELASTIC CALCULATIONS FOR MECHANICAL RELAXATION PHENOMENA DUE TO POINT DEFECT COMPLEXES IN METALS. Yoshiaki Kogure, Toshio Kosugi, Masao Doyama Teikyo University of Science and Technology.

A large number of mechanical relaxation peaks have been observed in the temperature dependence of internal friction in metallic crystals. The point defects or defect complexes responsible to the peaks are interstitials, impurity pairs, impurity-interstitial pairs and so on. These defects accompany a nonspherical strain field and respond to the external shear stresses. The temperature dependence of internal friction and elastic modulus change are used to be analyzed on the basis of phenomenological anelasticity model developed Nowick et al., in which the point defect strain per unit concentration is called as "the elastic dipole" and denoted by the λ- tensor. According to the model the magnitude of relaxation is proportional to the square of λ tensor. The relaxation time is the function of potential energy at a saddle point, and it can be calculated from the interaction potentials. Both the relaxation strength and the relaxation time for the point defects system in copper and aluminum alloys are calculated in this study. The atomistic displacement around the point defects and the saddle point energy are calculated by using the EAM potential based on the molecular dynamics simulation. The atomistic core region is surrounded by the elastic continuum region and both regions are connected on the basis of non-local elasticity theory. The interaction of elastic dipoles through the internal strain is also calculated to investigate the relaxation phenomena in glasses.

4:45 PM Z9.10
FIRST-PRINCIPLES QUANTUM MECHANICAL DESCRIPTION OF 100,000-ATOM MODELS OF ALLOY MICROSTRUCTURE. Alex Zunger, National Renewable Energy Laboratory, Golden, CO.

There is a lot of talk of computer-aided discoveries/design of new materials, but the simple fact is that even limiting oneself to materials made of just two elements, (e.g., Cu-Au or Si-Ge), and to a substitutional system there can exist as many as 2^N configurations that include compounds, alloys, superlattices, and impurities. Indeed, even for a modest number of sites N, this is an astronomical number. Thus, the conventional energy minimization approach for selecting the most stable crystal structure for $A_p B_q$ (e.g., first-principles pseudopotentials) is hopeless if one considers the full 2^N space configurations of A, B on a lattice of N points. Thus, contemporary energy minimization approaches use instead the method of "rounding-up the usual suspects": selecting the most stable from only a small number of well-known candidate structures. The potential for missing new and important structures is obviously large. Even if we know the stable structure at T = 0, we need to further know how it looks at finite-temperatures. This requires modeling short-range-order (SRO), precipitate morphology, etc. Computationally, this could need "supercells" with 10^4-10^6 atoms. This talk outlines the solution. It

addresses the questions of: (i) finding the lowest energy configuration of substitutional systems; (ii) calculating their composition-temperature phase diagram; and, (iii) their finite-temperature micro structure, including precipitate shapes and SRO, using the first-principles local density approximation (LDA). Mapping of the LDA energies of only 10-20 ApBq compounds onto an Ising-like "cluster expansion" enables use of lattice statistical mechanics techniques that elegantly solve the above problems. This extends the utility of the LDA from simple, perfectly-ordered compounds to truly complex structures. I will illustrate the method for semiconductor systems and transition-metal intermetallic systems, showing how previously unsuspected structures and materials are predicted, and how one can predict precipitate morphology (e.g., Al-Zn alloys).

SESSION Z10: THIN FILMS, CHEMISTRY
Chairs: Dieter W. Heermann and Scott M. Auerbach
Friday Morning, December 1, 2000
Independence W (Sheraton)

8:30 AM Z10.1
FACET: A TWO DIMENSIONAL SIMULATOR OF POLY-CRYSTALLINE THIN FILM GROWTH. Jie Zhang, James B. Adams, Arizona State University, Dept of Chemical and Materials Engineering, Tempe, AZ.

We present FACET: a two dimensional simulator to model polycrystalline thin film growth, linking atomic scale deposition and diffusion processes to macroscopic film growth. The model is based on the concept of describing the crystal surface in terms of preferred facets. Line segments are used to depict the profile of the grain and grain boundaries. Multiple nuclei are semi-randomly distributed along the textured or non-textured surface, and crystallographycally appropriate facets are created in the nucleation simulation. Both epitaxial and non-epitaxial growth can be simulated. We use the results of Kinetic Lattice Monte Carlo (KLMC) calculations to determine the inter-facet diffusion rates, which is an important input to FACET. A continuum approach is used to calculate facet growth rates based on the deposition and diffusion information. The code is run through an integrated Graphical User Interface for Windows (95/98/2000/NT). Users specify their simulation scale, deposition conditions, temperature, and crystal type (BCC and FCC currently available). Users then visualize the nucleation and growth of the film, and obtain the final grain structure and texture, all within a few minutes of simulation time on a typical PC. The code is freely available from our web site: http://ceaspub.eas.asu.edu/cms/

8:45 AM Z10.2
MULTISCALE MODELING OF PERITECTIC REACTION GROWTH. Marcel Ausloos and N. Vandewalle SUPRAS, Institut de Physique B5 Université de Liège, Liège, BELGIUM; R. Cloots, SUPRAS, Institut de Chimie B6 Université de Liège, Liège, BELGIUM.

A discussion of optical observations, models and simulations for the growth of materials at an incomplete peritectic reaction is presented. The emphasis is made on the role of reactive impurities, trapping and buoyancy. Theoretical models are solved in a Bethe lattice approximations. Applications to YBCO, a high critical temperature superconducting ceramics cuprate, is shown to be in good agreement with experimental data.

9:00 AM Z10.3
CALCULATION OF INTRINSIC STRESSES AND ELASTIC MODULI IN THIN FILMS. Pedro Andia, Francesco Costanzo, Gary L. Gray, Penn State University, Department of Engineering Science and Mechanics, University Park, PA.

The optical, electromagnetic and mechanical properties of thin films (TFs) are directly correlated to their morphology at the nanoscale. This, in concert with the fact that

- new deposition techniques are enabling the growth of thin films with very complex morphologies,

- there is an increasing interest in model-based simulation for the design of engineering structures (including nanostructures), and

- increasing computer speeds have given simulation an increasingly important role in the deposition of the thin films,

has made it increasingly important to understand how the nanostructure of a thin film impacts its properties at all length scales. In particular, creating a model-based simulation capability for the design of thin films will require the development of ways of predicting

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the nanostructure which results from a given set of deposition parameters (*e.g.*, substrate motion, deposition angle, ion bombardment, substrate temperature) as well as predicting the optical, electromagnetic, and mechanical properties of the resulting thin film. This paper is concerned with one aspect of the latter of these two issues, namely, the development of the capability of predicting some of the important mechanical properties of a thin film given that a simulation has been run which determines the locations of all the atoms (or clusters of atoms) in the thin film. We will describe variational techniques for the determination of elastic moduli in heterogeneous media (*e.g.*, both periodic and random composites). These techniques can be adapted for the determination of both the residual stresses as well as the elastic moduli of discrete media or, to be precise, of the continuum media which are mechanically equivalent to the discrete media of interest. The proposed technique is based on fundamental concepts of elasticity and is capable of capturing the variation of stresses and moduli as functions of position within the system.

9:15 AM Z10.4
STRESSES IN THIN COATINGS FROM CURVATURE MEASUREMENTS ON NON-PLANAR SUBSTRATES.
Adam Wikstrom and Peter Gudmundson, Royal Institute of Technology, Department of Solid Mechanics, Stockholm, SWEDEN.

Mechanical elastic and inelastic properties of thin films and patterned lines are often studied by means of the curvature measurement technique in combination with the Stoney formula. It is then implicitly assumed that the elastic substrate is initially flat. If the substrate have a slight initial curvature, a different situation arises. In this situation, the average stresses in the thin layer will remain constant over the surface but the measured curvatures will not. Therefore, measured curvatures can generally not be used to extract layer stresses without a proper compensation for the initial curvature. It is shown that through a simulation of curvature measurements it is possible to solve the inverse problem and hence to accurately compensate for the initial curvature. The corrected curvatures may then be used directly to determine average layer stresses through the Stoney formula. Explicit results are presented in closed form for a circular substrate with a spherical initial curvature and a generally non-elastic anisotropic thin coating. The results are particularly discussed in relation to curvature measurements on silicon wafers.

9:30 AM Z10.5
MODELING STRESS AND FAILURE IN SHRINKING COATINGS.
Herong Lei, Lorraine F. Francis, William W. Gerberich and L.E. Scriven, Coating Process & Fundamentals Program, Department of Chemical Engineering & Materials Science and Center for Interfacial Engineering, University of Minnesota, Minneapolis, MN.

Drying or curing of coating after vitrification or gelation is accompanied by stress development. Evaporation of solvent, polymerization and cross-linking, and cooling all cause shrinkage, but adhesion of the coating to the substrate prevents shrinkage to the stress-free state. The interaction of shrinkage and restraint creates strain and stress. If the local stress grows above the local strength of the coating, it can produce plastic yielding, cracking, delamination, or other defects. A large deformation elastic model is developed in order to analyze stress development in coatings subject to uniform shrinkage, the causes of which can be cooling, drying, reaction (as by UV-curing), or a combination of them. The solutions from the Galerkin/finite element method are used to analyze effects of free edges, delamination, and surface cracks. The solutions show highly concentrated stresses near the coating edge, and near the crack tips if the coating is delaminated or its surface is cracked. The elastic potential energy and strain energy release rate in both delamination and surface cracking are computed at different crack lengths. In both cases, results show that thicker coatings give larger energy release rate and thus are more vulnerable to cracking. The results also explain why there can be a critical coating thickness, the maximum thickness of coating that can remain crack-free. A crack can propagate only from an inherent flaw greater than a certain size. If the coating is thin enough that the maximum energy release rate is less than the crack growth resistance then no inherent flaws in the coating can grow into a crack, and so the coating remains crack-free.

10:15 AM Z10.6
TWO-LEVEL THERMOMECHANICAL MODEL OF A DIAMOND CRYSTALLIZATION IN A GRAPHITE-METAL MIXTURE AT HIGH PRESSURE AND TEMPERATURE. Alexander Leshchuk, V. Bakul Institute for Superhard Materials of the National Academy of Sciences of Ukraine, Kiev, UKRAINE.

The present paper deals with the numerical modeling of the diamond synthesis process in a high pressure apparatus (HPA). We consider the two scale levels: the whole HPA (first level) and the individual diamond crystal growing in the metal melt (second level). To describe

the process on the first level the numerical technique for FEM modeling of coupled nonlinear nonsteady processes of electrical and heat conduction and thermoplasticity, taking into account the large elastoplastic strains, phase transitions of materials and high pressure effect, has been developed. All equations are written for effective values of physico-mechanical properties. Phase transitions are determined from the changes in properties, concentrations and abrupt change in specific volume in the region where diamond synthesis is possible. For the second level, we take the following calculation scheme: a spherical diamond crystal surrounded by spherical layers of solvent-metal melt and graphite. The pressure and temperature at any point of reaction mixture determined from solving the problem for the first level is applied to outer surface of graphite. Then, the thermodynamic criterion of phase transition is entered, which takes into account inhomogeneity and nonhydrostatic character of the stress-strain state in the diamond-melt-graphite system and describes the area of transformations. The closed connection of solutions of the mechanical tasks at two scale levels is installed by the coordination of elastic modules of a reaction mixture and local diamond-melt-graphite system. A problem on determination of temperature, stresses and concentration fields in the reaction volume of HPA and in the local system under diamond synthesis conditions has been solved. The results demonstrate: a significant coupling of these fields; an interrelation of the solutions for the reaction mixture and for the local diamond-melt-graphite system; the effect of self-regulation of pressure in the HPA reaction zone consisting in pressure oscillation with respect to graphite-diamond phase transition line.

10:30 AM Z10.7
MULTISCALE MODELING OF MOLECULES IN NANOPORES: FROM SINGLE MOLECULE DYNAMICS TO CRITICAL PHENOMENA IN ZEOLITES. Scott M. Auerbach, Department of Chemistry and Department of Chemical Engineering, University of Massachusetts, Amherst, MA.

Zeolites are nanoporous crystalline aluminosilicates with a rich variety of interesting properties and industrial applications. As important as zeolites are industrially, the physics underlying their application is poorly known, in part because of the many length and time scales involved. To address these issues, we have applied a variety of simulation methods over many length scales to explore the jump dynamics, diffusion, orientational randomization and critical phenomena of benzene adsorbed in Na-X zeolite, because of persistent, qualitative discrepancies in the experimental literature for this system. We begin by discussing the computational challenges of calculating site-to-site jump rate coefficients using transition state theory with dynamical corrections. We then discuss kinetic Monte Carlo simulations of longer length scale benzene motion in Na-X, focusing on the virtues of fixed vs. variable time-step algorithms, as well as efficient treatments of adsorbate-adsorbate interactions. The results from these simulations are compared to a dynamic mean field theory we have developed for diffusion in zeolites. We then simulated benzene critical phenomena in Na-X using a two-replica cluster Monte Carlo algorithm, which exhibits very efficient equilibration. The critical temperature is found to vanish precipitously with increasing energy difference between sites, especially when high energy sites are favored entropically. We offer suggestions for efficient modeling of molecules in disordered nanopores, which require even further multiscale approaches.

10:45 AM Z10.8
A METHOD TO SIMULATE THE INTERFACE-DIFFUSION IN SOLID-STATE BONDING-PROCESSES CONSIDERING THE ELASTIC DEFORMATION. Takehiko Ito, Shigeki Saito, Kunio Takahashi and Tadao Onzawa, Department of International Development Engineering, Faculty of Engineering, Tokyo Institute of Technology, O-Okayama, Meguro-ku, Tokyo, JAPAN.

We propose a new method to simulate the interface-diffusion in the solid-state bonding-processes. This method is more significant for low pressure and low temperature conditions. It is available for the bonding of two bodies which consist of a kind of atoms and have rough surfaces. The rate of the bonding process is determined at least by four fundamental mechanisms; the plastic-deformation, the creep-deformation, the interface-diffusion and the volume-diffusion. Under low pressure, at low temperature, the interface-diffusion is dominant. The flux of the interface-diffusion depends on the stress distribution at the interface. It is important to know the elastic deformation in order to simulate the solid-state bonding-process. In a conventional method, the elastic deformation is not perfectly taken into account. The whole shape of the stress distribution is almost constant at the interface in the steady state, however, it changes dramatically in the transient state. Since the diffusion flux at the transient state is much larger than that of the steady state, the transient behavior can be used as a method to enhance the diffusion. It is thought that the bonding time could be shortened when the bonding pressure is changed at appropriate frequencies. The stress

distribution is considered and also the detachment of the surfaces at the edge of the contact regions is taken into account in the present method. In order to clarify the enhancement effect of various types of the pressure, three types of pressure application are examined, i.e., one is constant pressure, another is zero pressure, and the other is the on-off pressure. Our results suggest that the on-off pressure could decrease the required time for perfect contact if we could give an appropriate frequency of it to the process.

11:00 AM Z10.9
EFFECTIVE DETERMINATION OF COEXISTENCE CURVES USING REVERSIBLE-SCALING MOLECULAR DYNAMICS SIMULATIONS. <u>Maurice de Koning</u>, Sidney Yip, Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, MA; A. Antonelli, Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas, Unicamp, Campinas, São Paulo, BRAZIL.

An important application of atomistic simulation techniques concerns the prediction of the phase behavior of a given substance. The characterization of first-order phase transitions is particularly challenging in this regard, as a direct simulation of phase coexistence is usually difficult due to hysteresis effects related to the free-energy barrier separating the coexisting phases. In this work we present a simulation technique that allows the calculation of phase coexistence curves from a single, isothermal reversible-scaling molecular dynamics (MD) simulation. The approach is based on the simultaneous simulation of the two phases in separate cells and the integration of the corresponding Clausius-Clapeyron equation. Starting from a known coexistence point determined from prior free-energy calculations, the coexistence curve is traced out along a MD simulation of a nonequilibrium process to which both phases are subjected simultaneously. The process involves the time-dependent scaling of the potential energy function at constant temperature, while the temporal variation of the pressure is prescribed by the Clausius-Clapeyron equation. In contrast to other methods, this nonequilibrium procedure allows for the simultaneous determination of a coexistence curve and its associated chemical potential from a single and relatively short MD simulation. As an illustration of the effectiveness of our approach we apply the method to coexistence curves in the Lennard-Jones phase diagram.

11:15 AM Z10.10
MONTE-CARLO SIMULATIONS OF THREE DIMENSIONAL ION DYNAMICS IN POLYMERS. <u>A. Wagner</u>, H. Kliem, Saarland University, Institute of Electrical Engineering Physics, GERMANY.

Dynamic Monte-Carlo simulations of three dimensional ion motions are carried out based on a multiwell potential model. A parallel plate capacitor with an ionic conducting polymer dielectric having two ideal blocking electrodes is modeled. Positive ions (maximum 1000) are located on a cubic lattice with a maximum size of 50x50x100 locations. A negative background charge, constant in space and time, is used to provide charge neutrality. The positive ions can perform hops between neighbored sites with a probability corresponding to the energy barriers between the locations (hyper dynamics). It is assumed that the energy barriers between the allowed sites have an intrinsic distribution. The actual value of a barrier height is calculated from its intrinsic value, the contribution due to an applied field, and the contribution resulting from the field of all ions. To calculate this ionic field the method of images is used. For each ion the transition rate to one of the possible neighboring sites is calculated. With a Monte-Carlo (MC) step the ion, which actually moves, is determined. After this movement the new field distribution is calculated and the next hopping ion is determined using a further MC step. Thus our model yields a diffusive contribution and a field contribution. The dynamics of the ions are studied after application of an electric field step by computing the ionic current, the polarization response of the system, the internal electric field, and the space charge distribution. Two cases are considered: Quasi free ion movement between the electrodes and movement between two neighbored sites only, referring to a dipole ensemble. For the dipole ensemble we find the expected Debye relaxation for a single relaxation time and a polarization current $j(t) \propto t^{-1}$ for a box-like distribution of the intrinsic energy barriers. In the case of the quasi free ion motion and a single intrinsic relaxation time we find an exponential current with an ensemble relaxation time depending on the distance between the electrodes. For a distribution of intrinsic barrier heights we get a power law or a stretched exponential decay depending on the distribution. At small external fields and moderate ion densities a linear polarization can be calculated. In this case the external field is compensated by the field, which is generated by the displacement of the positive ions. At higher external fields the current is limited by the ion density. The ensemble relaxation time changes, and the polarization becomes nonlinear. A depletion layer at the positive electrode and an increased concentration of ions at the negative electrode is observed. Now the relaxation process is shifted towards a diffusion like behavior.