

SYMPOSIUM W

Modeling and Numerical Simulation of Materials Behavior and Evolution

April 2 – 5, 2002

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Proceedings to be published in both book form and online
(see *ONLINE PUBLICATIONS* at www.mrs.org)
as Volume 731
of the Materials Research Society
Symposium Proceedings Series

* Invited paper

SESSION W1: DISLOCATIONS AND PLASTICITY

Chair: Surya Kalidindi
Tuesday Morning, April 2, 2002
Golden Gate C2/C3 (Marriott)

8:00 AM W1.1

LINKING ATOMISTIC AND MESOSCALE MODELING OF PLASTICITY IN DYNAMIC FRACTURE. Robert E. Rudd, James Belak, Eira T. Seppala, Lawrence Livermore National Laboratory, Livermore, CA; Marc C. Fivel, CNRS/INPG, Grenoble, FRANCE.

We study the nucleation and growth of voids associated with dynamic fracture, with an emphasis on the concomitant plastic deformation and how information obtained at the atomistic level can be linked into dislocation dynamics simulation. The nanoscopic mechanisms of this high strain-rate plasticity have not been studied previously in detail. Large-scale molecular dynamics (MD) simulations have been used to characterize the dislocation structure and evolution during void growth in single crystal and polycrystal copper. The MD methodology for void growth developed by Belak [1] has been extended recently to allow on-the-fly characterization of dislocation activity at finite temperature in the plastic zone surrounding voids growing under tensile loading (cf. [2]). In a typical simulation, the initial configuration includes a pre-existing void. This system is brought to thermal equilibrium, and then a dilatational strain is applied that induces void growth. The resulting dislocation activity serves to transfer material away from the void, and is intimately associated with void growth. The role of prismatic dislocation loops has been studied in detail. We have further identified the character of the most numerous dislocations and their associated glide planes. This information is used to formulate a dislocation dynamics model of void growth for the single crystal case.

Acknowledgement:

This work was performed under the auspices of the US Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

[1] J. Belak, "On the nucleation and growth of voids at high strain-rates," *J. Comp.-Aided Mater. Design* 5, 193 (1998).

[2] R.E. Rudd and J. Belak, "Void Nucleation and Associated Plasticity in Dynamic Fracture of Polycrystalline Copper: An atomistic simulation," to appear in *Comput. Mater. Sci.* (2001).

8:15 AM W1.2

LINKING DISLOCATION DYNAMICS TO A CONTINUUM CRYSTAL PLASTICITY FORMULATION. Athanasios Arsenlis and Meijie Tang, Lawrence Livermore National Laboratory, Livermore, CA.

Advances in Dislocation Dynamics (DD) simulation methodologies over the past decade have not been reflected in working models of crystal plasticity at continuum length scales. The wealth of statistical information that these discrete dislocation line simulations generates has been not been effectively utilized to inform continuum models operating at larger a length scale. The classical hardening matrix-based formulations of single crystal plasticity at the continuum level are not well-suited to incorporate the microstructural information that the dislocation dynamics simulations provide. A new plasticity model called the Dipole Density Continuum Model is formulated to incorporate such microstructural information. The continuum model can be categorized as an internal state variable model in which the state is described by evolving densities of edge and screw dislocation dipoles on the crystallographic slip systems. The evolution equations for the dipole densities are developed from basic principles in dislocation mechanics such as the continuity of dislocation lines and conservation of Burgers vector. By treating the DD simulation cell as a representative volume element, DD simulation results are used to motivate the development of constitutive functions. Moreover, DD simulations are used to determine the material-specific parameters needed to quantify the plastic response of crystal and the accompanying evolution of dislocation density. A case study on the yield behavior of Tantalum single crystals is presented to demonstrate the ability of Dipole Density Continuum Model to capture the the dislocation density evolution and slip system activity predicted by DD.

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 No. W-7405-Eng-48.

8:30 AM W1.3

COUPLED ATOMISTICS AND DISCRETE DISLOCATION PLASTICITY. L.E. Shilkrot, Division of Engineering Brown University Providence, RI; Ronald E. Miller, Department of Mechanical and Aerospace Engineering, Carleton University, Ottawa, CANADA; W.A. Curtin, Division of Engineering Brown University Providence, RI.

Existing discrete dislocation (DD) techniques correctly describe long-ranged elastic interactions between dislocations without resorting

to a fully atomistic description; however they cannot capture atomic scale interactions, such as dislocation emission and crack growth in fracture, which are often important for a full understanding of the behavior. We present a multiscale coupled atomistic and discrete dislocation method (CADD) which overcomes this deficiency. In our approach, a material is divided into distinct regions which are treated either using fully atomistic approach or as a part of the material obeying continuum elasticity and populated by discrete dislocations. At the boundary between atomistic and continuum regions, continuity of tractions and displacements is maintained. Equilibrium for the coupled system is studied by finding the configuration of atomic and discrete dislocation positions that minimize the total energy of the system. The total energy is a sum of energies of atomistic regions, obtained by usual microscopic techniques, and the elastic continuum region containing discrete dislocations. The latter energy is found by the finite element analysis and with the use of the analytic continuum dislocation fields. An important feature of the model is the ability to detect when it is favorable for dislocations to move between the zones, and to automatically "convert" between the continuum and atomistic dislocation descriptions while rigorously maintaining compatibility across the interface. Several simple problems are solved that serve to demonstrate the validity, accuracy and efficiency of the CADD approach.

8:45 AM W1.4

100 DISLOCATION LOOP FORMATION AND CHARACTERIZATION IN FERRITIC MATERIALS: COMPARISON BETWEEN MODELING AND EXPERIMENTS. Jaime Marian, Brian D. Wirth, Lawrence Livermore National Laboratory, Chemistry and Materials Science Directorate, Livermore, CA; Robin Schäublin, CRPP, Fusion Technology-Materials, EPFL, Villigen PSI, SWITZERLAND; J. Manuel Perlado, Instituto de Fusión Nuclear, Universidad Politécnica de Madrid, Madrid, SPAIN.

Transmission electron microscopy (TEM) observation of irradiated ferritic materials reveals the existence of large, interstitial, dislocation loops with Burgers vectors $\frac{1}{2}(111)$ and (100) . These loops cause hardening of the material by pinning dislocations and impeding their glide during deformation. However, numerous molecular dynamics (MD) simulations of collision cascades in α -Fe have shown the exclusive formation of small, highly mobile, $\frac{1}{2}(111)$ clusters. Additionally, continuum dislocation theory and atomistic simulations have shown that $\frac{1}{2}(111)$ loops are energetically favored. This introduces the need to explain the mechanisms of formation and growth of (100) loops from small, cascade-produced clusters. The understanding of the physics underlying these phenomena is important for the development of solid damage accumulation models in ferritic materials that are being considered for fusion applications. In this work we propose a comprehensive set of dislocation reactions that explain the nucleation of (100) loops from $\frac{1}{2}(111)$ clusters. The growth up to TEM visible sizes of (100) loops through the absorption of one-dimensionally migrating $\frac{1}{2}(111)$ clusters is also assessed. (100) loops, although inherently glissile and higher in energy than $\frac{1}{2}(111)$ loops, are found to be thermally very stable and practically sessile with an activation energy for migration >3 eV. Finally, a direct comparison of TEM experimental micrographs with atomistic simulation-derived images is presented to show an example of how to help close the gap that exists between modeling and experiments.

9:00 AM W1.5

SIMULATIONS OF DISLOCATION DYNAMICS IN ALUMINUM INTERCONNECTS. Lucia Nicola, Erik Van der Giessen, Netherlands Institute for Metals Research, University of Groningen, Groningen, THE NETHERLANDS.

The stress that develops in aluminum interconnects due to thermal mismatch between line and substrate strongly affects interconnect reliability. Traditional treatments of stress relaxation rely on continuum approaches, but when the line width or height is smaller than a micrometer or so, the discrete nature of dislocations may no longer be ignored for an accurate prediction of local stress distributions. Therefore we choose to use discrete dislocation plasticity to study the build up and relaxation of stress in the section of single-crystalline, passivated aluminum lines placed periodically on a substrate. The approach treats dislocations in the aluminum interconnect as line singularities in an isotropic linear elastic medium. A set of constitutive rules is supplied for the glide of dislocations as well as their generation, annihilation and pinning at point obstacles. The solution for the state of stress and deformation is at every increment given as a superposition of two contributions: the known, analytical solution for individual dislocations in infinite space and a non-singular linear elastic, finite element solution that enforces the proper boundary conditions. The sum of these fields incorporates the long-range interactions. The numerical simulations track the evolution of the dislocation structure while thermal stress builds up. High concentrations of dislocations and therefore of stresses are predicted

at the line edges. The influence of the line aspect ratio will be studied as well as the effect of the line spacing.

9:15 AM W1.6

PARALLEL DISLOCATION DYNAMICS SIMULATIONS FOR PATTERN FORMATION. Wei Cai, Tim G. Pierce, Vasily V. Bulatov, Moon Rhee and Meijie Tang, Lawrence Livermore National Laboratory, Livermore, CA.

It has been envisioned that direct Dislocation Dynamics (DD) simulations can be used to predict plastic response of single crystals, particularly the strain hardening behavior and the associated evolution of dislocation microstructures. Unfortunately, this remains as a challenge to date. A representative simulation of the above processes requires integrating the motion of a large number (~ a million) of dislocation segments over a long period of time (sufficient to accumulate ~10% strain), which is beyond reach of the existing DD simulation codes. The bottleneck lies in the unfavorable scaling behavior of current DD codes with the number of processors, making them incapable of taking advantage of the massively parallel computing resources. In this talk, we present a new implementation of DD simulation that confronts this challenge. We discuss practical difficulties in dealing with line topologies, and describe new algorithms that handle them efficiently in parallel. Benchmark information of this new code will be presented, along with new results on spontaneous pattern formation by a large number of dislocations. This work is performed under the auspices of U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

9:30 AM W1.7

STOCHASTIC DISLOCATION DYNAMICS UNDER CREEP CONDITIONS IN METALS. Masato Hiratani, Hussein M. Zbib, Washington State Univ., MME, Pullman, WA.

A kinetic Monte Carlo algorithm is implemented into discrete dislocation dynamics code to investigate dislocation creep in a sub grain with local obstacles. This unification of stochastic thermal process with Newtonian mechanical process allows us to deal with problems of dislocation behavior over a wide range of stress and temperature regimes extensively without unphysical freeze of dislocation motions. In this code, the thermal activation rates of dislocations over the obstacles are calculated in terms of the elastic interaction energy depending on their relative orientation while pre-calculated data given by molecular dynamics are used when dislocation core reactions are involved. Copper with Frank Read sources and full stacking fault tetrahedra is chosen as a prototype for simulations under constant load. Results for strain rates reproduce both a conventional power law and the viscous controlled dependence below and above the critical resolved shear stress, respectively. In transient regions, the opposite temperature dependence of the thermal activation rates and phonon drags produces complex behavior of the flow stress due to the competition between softening and hardening. The contribution of dislocation inertial effect to obstacle bypass is also evaluated by checking the flight distance after an activation event. It turns out that the flight distance may be shortened by more than one order of magnitude without the inertia at very low temperatures. This result agrees with the experimental data indicating peculiar responses of the dislocation velocity such as a significant velocity reduction under strong magnetic fields in metallic single crystals.

10:15 AM *W1.8

SIMULATION OF NANO-SCALE CONTACT AT SURFACES. Subra Suresh, Massachusetts Institute of Technology, Dept of MS&E, Cambridge, MA.

The performance characteristics of many magnetic and electronic devices as well as the reliability of micro-electro-mechanical systems (MEMS) and nano-electro-mechanical systems (NEMS) can be strongly influenced by nanometer scale contact involving individual atoms, molecules or atomic scale asperities. In this presentation, we describe recent experimental simulations and molecular dynamics computational models of normal contact between surfaces of crystalline materials and nanoscale sharp or blunt indenters. The experimental simulations involve bubble raft models with atomically smooth surfaces or different scales of atomic-level roughness, as well as nanoindentation of monocrystalline and polycrystalline materials. Particular attention is devoted to the quantification of conditions governing the nucleation of defects for different surface conditions, crystallographic texture, or grain size of the nanostructured material. The experimental results are compared with multi-scale models covering the atomistic to the continuum length scales through discrete defect-level analyses. Experimental results of the effects of repeated nano-scale contact on the nucleation of defects at surfaces and the attendant roughening of surfaces and crack nucleation are also presented.

10:45 AM W1.9

ANALYSIS OF DISLOCATION JUNCTIONS IN FCC METALS. Laurent Dupuy, Rob Phillips, California Institut of Technology, Pasadena, CA; M.C. Fivel, Laboratoire GPM2-INPG, Saint Martin d'Hères, FRANCE.

The formation and strength of dislocation junctions in fcc crystals has been calculated using a line tension approach. In contrast to previous estimates, the concept of orientation-dependent line energy is explicitly considered. We first examine the structure of the different types of junctions existing in fcc metals in the absence of applied stress: Lomer-Cottrell lock, Hirth lock and glissile junctions. Far more interesting is their behaviour under stress: we have determined their 'yield surface' in stress space corresponding to their dissolution. Although the line tension model represents a huge simplification of the physics of dislocations, the comparison with more sophisticated models shows that it is able to satisfactorily reproduce the structure of junctions. In light of this success, we also examine the strength of junctions as a function of its geometry, namely, the length of the individual starting dislocations and their initial orientation with respect to the line of intersection of the two glide planes. The results from this simple model can provide useful parameters related to junction strength in higher level models of single crystal plasticity.

11:00 AM W1.10

ON THE INTERACTION BETWEEN Mg SOLUTE ATOMS AND DISLOCATIONS IN Al-Mg ALLOYS. Catalin Picu, Dawei Zhang, Rensselaer Polytechnic Institute, Department of Mechanical, Aerospace and Nuclear Engineering, Troy, NY.

The interaction between solute atoms and dislocations is known to lead to negative strain rate sensitivity and poor formability. The negative rate sensitivity leads to inhomogeneous flow and the Portevin-LeChatelier effect. These observations motivate the present study of the details of the solute-dislocation interaction in binary Al-Mg alloys. The analysis is based on atomistic simulations. It is shown that Mg atoms form small clusters in Al in absence of any lattice defect. The clustering process is favored by a temperature decrease and by a homogeneous tensile hydrostatic stress. Other stress components are seen to have a small effect on the clustering process. In presence of an inhomogeneous strain field, e.g. about a stationary dislocation, clustering is more pronounced. The temperature and stress dependence of this process is studied. Finally, the Peierls stress of the decorated dislocation is determined as a function of cluster size.

11:15 AM W1.11

ATOMISTIC SIMULATION OF DISLOCATION-GRAIN BOUNDARY INTERACTIONS. M. de Koning, W. Cai, V.V. Bulatov, Lawrence Livermore Natl. Lab, Livermore, CA.

Predictive modeling of polycrystal plasticity requires an atomistic-micro-meso scale computational approach in which the physics of individual defects such as dislocations and grain boundaries (GB) is incorporated in microscale models of the evolution of large collections of them and, ultimately, in mesoscale models of the aggregate behavior of grain microstructures under stress. A fundamental step in the construction of such a model concerns the understanding of the basic plasticity mechanisms involving the interactions between dislocations and grain boundaries. In the present paper we employ atomistic simulations to examine such interactions in a bicrystal of aluminum. We conduct a series of molecular dynamics (MD) simulations in which a dislocation dipole is placed in the vicinity of a grain boundary separating both grains. We discuss the influence of various involved parameters, including the GB geometry, applied stress conditions and temperature. This work is performed under the auspices of U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

11:30 AM W1.12

AN ANALYSIS OF GRAIN BOUNDARY STRENGTHENING BEHAVIOR BY USING DISCRETE DISLOCATION DYNAMICS. S.B. Biner and J.R. Morris, Ames Laboratory, Iowa State University, Ames, IA.

In this study, the evolution of the flow stress for grain sizes ranging from about 16 to 2 μ m under shear deformation was simulated using a two dimensional discrete dislocation dynamics. The analyses were confined to a single slip system and to the collective behavior of large number of edge dislocation. A superposition technique, combined with Boundary Element Method, was used to obtain the solution resulting from the dislocation microstructures and kinematic boundary conditions. The long-range interactions of dislocations were fully accounted for with the Multi-Pole Algorithm without introducing an artificial length scale in the form of a cutoff radius. We observe an increase in the flow stress values with decreasing grain size. We also see that dislocation pileups can both activate neighboring dislocation

sources and also shutdown the active dislocation sources. Flow stress values are correlated with grain size in the form of classical Hall-Petch relationship $[d]^{-1/2}$, however, a similar correlation was also observed when they are correlated with grain size in the form of $[d]^{-1}$. The effects of the multi-slip and grain size distributions on the deformation and strengthening behavior are also elucidated for selective cases. This work was performed for the United States Department of Energy by Iowa State University under contract W-7405-Eng-82. This research was supported by the Director of Energy Research, Office of Basic Sciences.

11:45 AM **W1.13**

SOLUTE STRENGTHENING OF BCC ALLOYS: KINETIC MONTE CARLO SIMULATIONS OF DISLOCATION MOTION IN A SOLUTE FIELD. Chaitanya Deo, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI; Department of Mechanical and Aerospace Engineering, Princeton University, Princeton NJ; David J. Srolovitz, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton NJ; Wei Cai, Vasily Bulatov, Chemistry and Materials Science Directorate, Lawrence Livermore National Laboratory, Livermore, CA.

The interaction of dislocations and solute atoms is key to understanding crystal plasticity in alloys. We present a kinetic Monte Carlo (kMC) simulation of the glide of a $\langle 111 \rangle$ screw dislocation on the (011) plane in body centered cubic molybdenum in the presence of substitutional solute atoms. The dislocation motion is described in terms of a kink model, which explicitly includes double kink nucleation, kink migration and kink-kink annihilation. The barriers for double kink nucleation and kink migration are obtained from atomistic simulations. Since double kink nucleation is much slower than kink migration in bcc metals, most of the simulation time would normally be used to form double kinks. To increase the simulation efficiency we integrate over the initial evolution of the embryonic double kink by treating the growth as a one-dimensional random walker and obtaining the distribution of the elapsed time before the double kink stabilizes. The time distribution is obtained by applying an exact first passage time analysis for temporally homogenous discrete state Markov processes to the one-dimensional random walk of the embryonic double kink that nucleates on the dislocation. Incorporation of such a double kink nucleation model is a key to efficient simulations. We perform simulations at several solute concentrations and a range of stresses. We observe the evolution of the dislocation shape and determine the threshold for continuous dislocation motion as a function of applied stress and solute concentration. The stress-plastic strain rate relationships are investigated as a function of solute concentrations.

SESSION W2: MODELING OF MATERIALS RESPONSE

Chair: Michael V. Braginsky
Tuesday Afternoon, April 2, 2002
Golden Gate C2/C3 (Marriott)

1:30 PM ***W2.1**

MESOSCALE MODELING OF HOT SPOT FORMATION IN ENERGETIC MATERIALS. David Benson, University of California, San Diego, CA; Philip Howe, Los Alamos National Laboratory, Los Alamos, NM.

Detonation is initiated in energetic materials by the formation of regions of localized heating called "hot spots." Understanding the formation and distribution of hot spots within an energetic material is crucial to understanding its behavior and how to design safer energetic materials. Previous work has focused on HMX powders as a model for damaged energetic materials, while the current work focuses on an idealized polymer bonded explosive (PBX) that is devoid of the structural imperfections (e.g., voids) usually proposed as hot spot formation sights. Synthetic microstructures have been generated for PBX-9501, an energetic material composed of 95% HMX and 5% binder. The particle size distributions are bi-modal, with particle size ratios of 2:1 and 4:1. The largest particles have a nominal diameter of 100 microns. Particle velocities ranging from 0.5 km/s to 3.5 km/s are imposed and the temperature distribution is calculated after the first shock has passed through the microstructure. Among the interesting results is the formation of long, heated segments along the grain boundaries that are approximately parallel to the shock direction.

2:00 PM **W2.2**

ATOMIC-SCALE VOID GROWTH SIMULATIONS USING COUPLED ATOMISTICS AND DISCRETE DISLOCATION PLASTICITY. Ronald E. Miller, Department of Mechanical and Aerospace Engineering, Carleton University, Ottawa, CANADA; L.E. Shilkrot and W.A. Curtin, Division of Engineering, Brown University, Providence, RI.

Recently, we have developed the coupled atomistic and discrete dislocation plasticity (CADD) approach, whereby we model some regions of a problem using full atomistics and others using a discrete dislocation plasticity description. In this research, the technique is used to study the details of atomic-scale void growth mechanisms in ductile metal crystals. CADD fills an important gap in our ability to bridge the length scales when modeling dislocation-mediated deformation phenomena like void growth. By combining the strengths of atomistic models with those of the discrete dislocation approach, the new model overcomes the shortcomings of both techniques. Experimental evidence [1,2] has shown that small voids growing due to plastic deformation often have growth rates that significantly exceed the predictions of continuum void growth models. What is lacking in the continuum models is the correct description of the anisotropy of slip in single crystals and the atomic-scale details of how dislocations are nucleated at the void surface. In this work, we will develop an understanding of how these effects contribute to the observed higher growth rates. The CADD technique allows us to "measure" void growth rates for a variety of virtual crystals, and then study in detail the mechanisms of void growth. Further, CADD facilitates a systematic investigation of how these mechanisms are affected by pre-existing dislocations in the crystal. One aspect of void growth on which we focus is dislocation nucleation. Recently, Acharya [3] has proposed the intriguing notion that the curl of stress at a point should be used in a nucleation criterion. This idea stems from a non-local continuum mechanics formulation, and is a radical departure from the usual nucleation criteria based on stress or strain. The CADD method allows us to test Acharya's claim in the context of dislocation nucleation during void growth.

References:

- J. Crepin, T. Bretheau and D. Caldemaison, "Cavity growth and rupture of beta-treated Zr: a crystallographic model," *Acta Mater.*, Vol. 44, No. 12, pp.4927-4935 (1996).
J. Crepin, T. Bretheau and D. Caldemaison, "Plastic deformation mechanisms of beta-treated Zr," *Acta Metall. Mater.*, Vol. 10, pp. 3709-3719 (1995).
A. Acharya, "Driving forces and boundary conditions in continuum dislocation mechanics," submitted for publication (2001).

2:15 PM ***W2.3**

MICROSTRUCTURE DESIGN AND OPTIMIZATION USING SPECTRAL REPRESENTATIONS: NOVEL TOOLS FOR THE MATERIALS ENGINEER. Surya R. Kalidindi, Josh Houskamp, Drexel University, Dept of Materials Engineering, Philadelphia, PA; Brent L. Adams, Brigham Young University, Dept of Mechanical Engineering, Provo, UT; and Hamid Garmestani, FAMU-FSU College of Engineering, Tallahassee, FL.

The authors have recently developed and reported a new paradigm to facilitate materials by design by using spectral representations of microstructure and the associated properties. In this paper, the tremendous advantages of using the spectral method in describing the universe of all relevant microstructures for the design problem at hand (denoted as the material hull) and the space of all physically realizable property combinations (denoted as the property closure) will be described. The paradigm will then be extended to include considerations of process design that is predicted to result in pre-selected microstructures. It will be shown that there are significant advantages to describing microstructure evolution in the Fourier space. Specifically, the concept of streamlines has been used to mathematically represent both the microstructure evolution in the material hull and the concomitant property evolution in the property closure. The newly developed methodologies will be demonstrated in the context of a specific design example.

2:45 PM **W2.4**

FURTHER INVESTIGATION AND APPLICATION OF THE PRINCIPLE OF CORRESPONDENCE BETWEEN ELASTIC AND PIEZOELECTRIC PROBLEMS. Edgar Karapetian, Suffolk University, Dept. of Mathematics and Computer Science, Boston, MA; Larissa Gorbatiikh, University of New Mexico, Dept. of Mechanical Engineering, Albuquerque, NM.

In the present work, the recently established principle of correspondence between the elastic and the piezoelectric problems for the transversely isotropic materials has been applied to obtain the solution of the problem of interaction of two tangential forces and a penny-shaped crack. The problem under consideration is described as follows: a penny-shaped crack in the unbounded piezoelectric medium is loaded by a pair of equal and opposite point forces that are tangential to the crack and are applied symmetrically with respect to the crack plane which is a plane of isotropy. Some further investigation of the principle of correspondence is made and the important limiting conditions are stated. The implementation of these limiting conditions is illustrated on few examples.

3:30 PM W2.5

STRESS CALCULATION IN ATOMISTIC SIMULATIONS OF PERFECT AND IMPERFECT SOLIDS. J. Cormier, Lehigh Univ., Dept. of Mechanical Eng., Bethlehem, PA; J.M. Rickman, Lehigh Univ., Dept. of Matl. Sci. & Eng., Bethlehem, PA; T.J. Delph, Lehigh Univ., Dept. of Mechanical Eng., Bethlehem, PA.

Lutsko (J. Appl. Phys. **64**,1152, 1988) has shown how the equation expressing conservation of linear momentum on the atomic level may be solved to yield a closed form expression for the local stress tensor. We analyze in detail a volume-averaged version of this stress tensor. For spatially inhomogeneous stress fields, this volume-averaged result merges smoothly with the continuum stress tensor for sufficiently large averaging volumes. Computed results for an inclusion in an FCC crystal are presented. Good agreement is found with the continuum stress field up to a few atomic spacings from the inclusion. At distances closer to the inclusion, the continuum solution begins to break down. Considerably poorer agreement was noted with the commonly-used atomic stress tensor, which is strictly valid only for spatially constant stress fields.

3:45 PM W2.6

A NEW LOOK AT THE ATOMIC LEVEL VIRIAL STRESS-ON CONTINUUM-MOLECULAR SYSTEM EQUIVALENCE. Min Zhou, The George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA.

As one of the most commonly used definitions of stress in discrete molecular systems, the virial stress includes two parts. The first part depends on the mass and velocity of atomic particles, reflecting an assertion that mass transfer causes mechanical stress to be applied on stationary spatial surfaces external to an atomic particle system. The second part depends on interatomic forces and atomic positions, providing a continuum measure for the internal mechanical interactions between particles. The virial stress violates balance of momentum and does not possess physical significance as a measure for mechanical interaction between material points. The lack of physical significance is both at the individual atom level in a time-resolved sense and at the system level in a statistical sense. As a stress-like quantity, the virial stress has the geometric interpretation of being a measure for momentum change in a fixed spatial region. It is demonstrated that the interatomic force term alone is a valid stress measure and can be identified with the Cauchy stress. The discussions focus on an error in the theoretical derivation of the virial stress that led to the inclusion of the kinetic energy term and on the conceptual flaws in the argument commonly used for including it. To further illustrate the irrelevance of mass transfer to the evaluation of stress, an equivalent continuum (EC) for dynamically deforming atomistic particle systems is defined. The equivalence of the continuum to discrete atomic systems includes (i) preservation of linear and angular momenta, (ii) conservation of internal, external, and inertial work rates, and (iii) conservation of mass. This equivalence allows fields of work- and momentum-preserving Cauchy stress, surface traction, body force, and deformation to be determined. The resulting stress field depends only on interatomic forces, providing an independent proof that as a measure for internal material interaction stress is independent of kinetic energy or mass transfer.

4:00 PM W2.7

NON-LOCAL ELASTICITY KERNELS EXTRACTED FROM ATOMISTIC SIMULATIONS. Catalin Picu, Rensselaer Polytechnic Institute, Department of Mechanical, Aerospace and Nuclear Engineering, Troy, NY.

The kernel of the integral formulation of linear non-local elasticity is determined from atomistic simulations. To this end, glasses of several materials are prepared by molecular simulation techniques, and a procedure is devised by which the continuum constitutive model is calibrated based on the numerical results. Both model (Lennard-Jones and Morse) and realistic (Aluminum) materials are considered. The role of various features of the interatomic potential in determining the shape of the non-locality kernel is investigated in the Morse solid. The functional form of the kernel is different than that usually assumed within the integral formalism (Gaussian), exhibiting a significant negative region. Furthermore, the assumption that a unique kernel may describe all elastic constants of a given solid is not justified based on the present simulation results. The new kernels have a range (internal length-scale) comparable with the potential cut-off, are able to represent wave dispersion near the Brillouin zone boundary, and to mimic surface energy effects. They also provide improved predictions of the Peierls stress of a dislocation within the Peierls-Nabarro model.

SESSION W3: MOLECULAR DYNAMICS AND AB-INITIO MODELS

Chair: Eugene Olevsky
Wednesday Morning, April 3, 2002
Golden Gate C2/C3 (Marriott)

8:00 AM W3.1

TOPOLOGICAL MOLECULAR DYNAMICS MODELING OF A CHEMICAL DISORDER THRESHOLD IN THE AMORPHIZATION TRANSITION OF CRYSTALLINE SILICON CARBIDE. Xianglong Yuan, Linn W. Hobbs, Department of Materials Science & Engineering, Massachusetts Institute of Technology, Cambridge, MA.

Silicon carbide (SiC) is a promising blanket material for nuclear fusion reactors, inert matrix for transmutation of Pu, and wide-gap semiconductor for device applications in severe environments. The difficulty of diffusion doping favors ion implantation routes for electronic device manufacture using this material. Of particular interest in all these applications is the irradiation-induced amorphization of SiC, which turns out to be as easy as silica or silicon, surprising result given the rigidity constraints on the structure, which involve four [SiC₄] tetrahedra sharing every tetrahedron vertex. We have explored the role of chemical disorder (Si substituting for C and vice versa) on the amorphizability of SiC by introducing set levels of chemical disorder (defined by the homopolar bond concentration) into initially perfectly crystalline arrangements and subsequently equilibrating the ensemble with molecular dynamics routines at temperatures between 100 K and 7000 K. We have discovered a homopolar bond threshold (systemically about 40%), below which equilibrated structures retain long-range order and exhibit a melting transition, and above which the system amorphizes and undergoes a further glass transition at about 3000 K. The result explains the ease of SiC amorphization, attributable to the fact that the replacement sequences and Frenkel disorder accompanying radiation-induced displacements locally contribute a homopolar bond concentration above the threshold value. The transition may additionally be driven by an observed larger attendant Si coordination than 4. Most of the observed dimensional change is, however, attributable to earlier stages of chemical disorder.

8:15 AM W3.2

A DFT STUDY OF STRUCTURE AND PROPERTIES OF AMORPHOUS SiCN. Peter Kroll, Institute of Inorganic Chemistry, RWTH Aachen, GERMANY.

We investigate structure and properties of amorphous silicon carbonitride materials using density functional methods. Topologically different models of a-SiCN with 100-200 atoms each were generated from continuous alternating random networks. The networks have distinct topologies which results in a different chemical bonding in the investigated structural models. A first series of models consists of Si-N and C-N bonds only and is an intermediate between a-Si₃N₄ and a-C₃N₄. We found that a tetrahedral coordination of "cationic" carbon in such compounds is unstable at elevated temperatures, as indicated by Car-Parrinello molecular dynamic (CPMD) simulations. A second series of models consists of Si-N and Si-C bonds only and therefore are in-between a-Si₃N₄ and a-SiC. For such materials with "anionic" carbon we found the highest elasticity coefficients. However, the network strain increases with increasing SiC content, resulting in Si-C bond rupture and bond redistribution in the amorphous structure. A third series of models consists of amorphous Si₃N₄ as host structure and segregations of graphitic C in pores and cavities. Vibrational spectra of such models might be useful for phase characterizations due to the presence of d- and g-bands.

8:30 AM W3.3

UNDERSTANDING ORDER IN SILICON USING ACCELERATED MOLECULAR DYNAMICS ALGORITHMS. Devashish Choudhary, Paulette Clancy, School of Chemical Engineering, Cornell University, Ithaca, NY.

The electronic properties of silicon phases are inextricably linked to the underlying order in the material: Liquid silicon is metallic in nature, whereas amorphous and crystalline silicon are semiconducting. The existence of a metallic supercooled glassy silicon is unknown; the quench rate window available to experiments is too low to observe this material, except perhaps transiently. In computational studies, the problem is reversed: The time scale accessible to Molecular Dynamics is too small (order of nanoseconds) to study the evolution of amorphous silicon from the relaxation of an ultra-rapidly quenched liquid. Such studies require methods like Hyper-Dynamics^{1,2} (HMD) and Self-Guided Molecular Dynamics³ (SGMD) that reduce the effects of frequent, but non-essential, events. We have implemented both HMD and SGMD algorithms for an empirical Stillinger-Weber (SW) potential and checked the effect of key parameters on the system performance. From a liquid state, silicon was quenched at 10¹¹ K/s to a temperature of 700 K and allowed to evolve in a NPT

(isobaric-isothermal) ensemble for a period of ~ 50 ns, observing any structural changes that occurred. Important new insight was provided by an order parameter⁴ based on a pattern recognition technique. Determination of the electronic and thermodynamic properties throughout this evolution, obtained using quantum mechanical methods, showed that these properties are closely linked with the structural changes taking place. Most of the final structural properties using HMD and SGMD were found to be identical. The average coordination number of the final structure fluctuates around 4.10 (c.f. experimental value: 3.88 and continuous random network (CRN) model: 4.0). Minimization of the final SW configuration using a tight-binding algorithm yielded a sample with a coordination number of 3.97 having structural and electronic properties very similar to that of the CRN model and experiment.

References:

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8:45 AM W3.4

AB INITIO BASED MODELING OF III-V SEMICONDUCTOR SURFACE PROPERTIES. Frank Grosse and Mark F. Gyure, HRL Laboratories, Malibu, CA.

The predictive capability of calculations employing ab initio density functional theory (DFT) allows investigating electronic and structural properties on the atomic scale with high accuracy. Complex behavior like growth on III-V semiconductor surfaces is however influenced by a number of different atomic processes. Numerical demand of DFT calculations does not allow very often a direct investigation of growth processes. Insight gained by DFT calculations can be combined in models bridging to length and time scales of interest and at the same time keeping the accuracy of DFT. We will demonstrate the application of a DFT based kinetic Monte-Carlo simulation (KMC) on InAs(001) growth on vicinal surfaces. A large number of energies calculated by DFT for reconstructions, adsorption energies for single and multiple In adatoms and As-dimers, and As desorption pathways are used to construct the KMC model energy. We achieve an accuracy of the model energy comparable to the accuracy of the DFT calculation itself. Application of the KMC simulation to growth on vicinal surfaces with A (along $[110]$) and B steps (along $[\bar{1}10]$) reveals the reason for the difference in the transition temperature to step flow mode which is higher on surfaces with A steps. We trace the experimentally observed behavior back to the atomic difference in nucleation which is a direct consequence of the different atomic structure of the steps.

9:00 AM W3.5

PHASE TRANSFORMATIONS ON CATION INTERCALATION IN ANATASE FROM FIRST PRINCIPLES. Marina V. Koudriachova^a, Nicholas M. Harrison^b and Simon W. de Leeuw^a. ^aComputational Physics, TU Delft, Delft, THE NETHERLANDS. ^bCLRC, Daresbury Laboratory, Daresbury, Warrington, UNITED KINGDOM.

Anatase structured titania is a prospective electrode material in high energy density Li-rechargeable batteries. It is also tested widely for applications in solar cells and electrochromic devices. Though anatase is currently used as an anode in commercial batteries, the mechanism of Li-intercalation is not well understood. Here we present results of first principles calculations of Li-intercalation into anatase structured titania. The computed data are summarized in a model of diffusion limited intercalation, which accounts for all known experimental data and their temperature dependence. We correctly predict a phase transformation to the orthorhombic phase and discuss the mechanism of the phase transition. The structure of Li-anatase is affected by deformations due to the size of Li-ions and due to the donation of the electronic charge which accompanies Li-intercalation. The influence of the size of the guest ion was separated by considering structures containing He, H, Na and K -atoms in addition to Li. We show that transformation to the orthorhombic phase can be completely explained in terms of charge localization and the size of Li-ions. The optimal structures for H- and Na-anatase, though very different from that of Li-anatase, were also found to be orthorhombic. For Na ions with the much larger ionic radius we predict another phase transformation to a layered phase. We show that locally the changes of the structure can be fully interpreted in terms of size of the guest ion. We also consider the influence of geometry of the host lattice on the distribution of the donated electronic charge by computing different polymorphs of Li-titania. The global charge distribution does not significantly depend either on the structure of the host or on the

nature of the guest cation. The distribution is essentially the same for all stable configurations considered, which indicates that it is fully determined by electronegativities of the framework atoms.

9:15 AM W3.6

TRANSFORMATION OF γ -Al₂O₃ TO θ -Al₂O₃. Shuhui Cai^{1,2}, Karl Sohlberg². ¹Department of Physics, Xiamen Univ, Xiamen, PR CHINA. ²Department of Chemistry, Drexel Univ, Philadelphia, PA.

γ - and θ -Al₂O₃ are two common metastable polymorphs of aluminum oxides. These polymorphs can be observed along the dehydration sequence of boehmite upon thermal treatment before conversion to the final product α -Al₂O₃. Analysis of their crystal structures shows that, both of them can be nominally redefined to crystal cells with formula Al₁₆O₂₄ which have similar lattice parameters (assuming two vacancies every Al₁₆O₂₄ for γ -Al₂O₃). Comparing these two cells, we find that when some of the aluminum atoms in γ -Al₂O₃ move to specific 16c and 48f sites, a close approximate of θ -Al₂O₃ is formed. First principles total energy calculations have been carried out on this and related structures. The approximate and experimental θ -Al₂O₃ optimize to the same structure within the margins of error of the model. (They differ in total energy by 0.0025 eV/Al₂O₃). There are four possible direct paths for the migration of aluminum atoms to the nearby interstitial sites of the oxygen-anion subcell in γ -Al₂O₃ to become θ -Al₂O₃: I. 8a to 16c; II. 16d to 48f; III. 8a to 48f; IV. 16d to 16c. The energy differences between the states before and after the migrations have been computed and were found to be related to the positions of cation vacancies. Taking the transformation temperature into account, the migration may take place in the vicinity of cation vacancies first to reduce strong Al-Al interactions. The migrations of the remaining aluminum atoms start when new vacancies are produced near their destinations. By this procedure, 8b sites of γ -Al₂O₃ do not need to be involved. This means that it is possible for γ -Al₂O₃ to transform to θ -Al₂O₃ without being formally disordered to a simple fcc structure first.

9:30 AM W3.7

ISOSTRESS MOLECULAR-DYNAMICS STUDIES OF MECHANICAL INSTABILITY, PHASE CHANGE, AND FAILURE IN CRYSTALS UNDER STRESS. Jianhua Zhao, Robert S. Hoy, Dimitrios Maroudas and Frederick Milstein, University of California, Santa Barbara, CA.

Mechanical, geometric, and kinetic characteristics of instabilities in crystals under stress are revealed via isostress molecular-dynamics (MD) simulations according to the Lagrangian formulation of Parrinello and Rahman. Special emphasis is placed on bifurcations exhibited along the crystals primary deformation path as the applied load is varied. Particular attention is given to the topics of (i) elastic instabilities at points of bifurcation (as predicted by the elastic stability criteria of Hill and Milstein), (ii) post bifurcation phenomena leading to phase change or material failure, and (iii) crystal symmetry, which strongly influences the mechanical response and bifurcation behavior. Fluctuation formulae are used for computation of elastic moduli employed in assessments of elastic stability. Interatomic interactions are expressed by pair potentials that have been fitted to experimental elastic moduli of metals. No special significance is placed on the specific forms of interatomic potentials, since our main concern is qualitative mechanistic understanding of stress-induced elastic instabilities in crystals; however, the potentials do, in fact, yield large-strain behavior in excellent qualitative agreement with more rigorous atomistic models and with experiment. The MD calculations are made over wide ranges of temperature and stress, for various modes of applied load, including uniaxial loads along the major crystallographic axes. The observed instabilities are found to be thermally activated and are associated with vanishing or diminishing elastic moduli combinations.

10:15 AM W3.8

DIRECT SIMULATION MONTE CARLO CALCULATION: STRATEGIES FOR USING COMPLEX INITIAL CONDITIONS. Michael I. Zeifman, Barbara J. Garrison, Department of Chemistry, The Pennsylvania State University, University Park, PA; Leonid V. Zhigilei, Department of Materials Science and Engineering, School of Engineering and Applied Science, University of Virginia, Charlottesville, VA.

Modeling of phenomena is increasingly being used to obtain an understanding of important physical events as well as to predict properties that can be directly tied to experimental data. For systems with relatively low densities of particles, the Direct Simulation Monte Carlo (DSMC) method is well suited for modeling gases with non-equilibrium distributions, coupled gas-dynamic and reaction effects, emission and absorption of radiation. On the other hand, if the density of particles is large such as in dense gases or condensed matter, the DSMC method is not appropriate and techniques such as molecular dynamics (MD) simulations are employed. There are

phenomena such as laser ablation, however, in which the system evolves from a condensed state appropriate to be studied with MD to an expanding rarified gas appropriate to be studied with DSMC. The work presented here discusses the means of transferring information from a MD simulation of laser ablation to a DSMC simulation of the plume expansion. The presence of clusters in the MD output poses the main computational challenge. When the laser fluence is above the ablation threshold, the cluster size distribution is very broad (up to 10,000's of particles per cluster) but there are relatively few of each cluster size. We have developed a method for statistical processing of the MD results and have represented the cluster size as a random variable. Various aspects of the coupling between the MD and DSMC models are discussed and several examples are presented.

10:30 AM W3.9

HYBRID MODEL SIMULATION ON CLUSTER GROWTH AND DEPOSITION PROCESSES. Hiroshi Mizuseki, Kenta Hongo, Yoshiyuki Kawazoe, Institute for Materials Research, Tohoku University, Sendai, JAPAN; Luc T. Wille, Department of Physics, Florida Atlantic University, Boca Raton, FL.

Magnetic films obtained by cluster deposition have attracted strong attention both as a new manufacturing technique to realize high density magnetic recording media (1) and to create systems with unique magnetic properties. Since the film's features are influenced by the cluster properties during the flight path, the relevant physical scale to be studied is as large as centimeters. Moreover, since the behavior of segregation processes on the substrate is not negligible, the smallest physical scale is of the order of 10 nm. Although a complete analysis of this multiscale problem is extremely difficult, it provides a typical research subject in the dynamics of a complex system consisting of interacting subsystems with very different scales. In this paper a new model of cluster growth and deposition processes based on a combination of Direct Simulation Monte Carlo (DSMC) (2) and Monte Carlo (MC) methods is introduced to examine the effects of experimental conditions on film formation by an adiabatic expansion process. From the macroscopic viewpoint, we simulate the behavior of clusters and inert gas in the flight path under different experimental conditions. The internal energy of the cluster, which consists of rotational and vibrational energies, is limited by the binding energy which depends on the cluster size. This binding energy is obtained by classical molecular dynamics. Several types of size distributions of generated clusters under various conditions are obtained by the present model. The results of the simulations show that the size distribution is strongly related to the experimental conditions and in turn has a major effect on the film properties.

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10:45 AM W3.10

FUNDAMENTAL GRAIN BOUNDARY PROPERTIES FOR MODELLING RECRYSTALLIZATION IN ALUMINUM.

M. Upmanyu, Computer Science and Mathematics Division, Oak Ridge National Laboratory and Materials Science Program, Division of Engineering, Colorado School of Mines; H. Zhang, D.J. Srolovitz, Department of Mechanical and Aerospace Engineering, Princeton University and A. Rollett, Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA.

Anisotropic grain boundary properties such as intrinsic mobilities and energies (both excess free energy of the grain boundary and the activation energy for migration) are important for our understanding of fundamental metallurgical phenomena such as grain growth and recrystallization. We present results of atomistic simulation studies using molecular dynamics to extract these boundary properties in pure aluminum. The simulations were performed on individual grain boundaries in 3-dimensions using a half-loop bicrystal geometry and the well known EAM potential for Al (Voter-Chen). The large phase space associated with boundary crystallography in such calculations is circumvented by focussing on a few key grain boundary bicrystallographies that are important for recrystallization of Al. Key relationships such as the cube component ($\{001\}\langle 100 \rangle$) against the copper component ($\{112\}\langle 111 \rangle$) are important for our understanding of the formation of strong annealing textures. Certain components of a deformation texture such as $\{123\}\langle 634 \rangle$ are thought to have high mobility interfaces with the cube component thereby enabling rapid growth of the latter texture. This investigation also serves to extend the simulation of grain boundary properties beyond the highly symmetric sets based on misorientations about $\langle 111 \rangle$ and $\langle 100 \rangle$ that are available in the literature. They will also provide much needed information on constitutive properties for mesoscale simulations of grain growth and recrystallization.

11:00 AM W3.11

FIRST PRINCIPLES PREDICTIONS OF THE STRUCTURE AND

BONDING AT IRON-CERAMIC INTERFACES. A. Arya and Emily A. Carter, Department of Chemistry and Biochemistry, UCLA, Los Angeles, CA.

Ceramics possess an unusual combination of physical, chemical and mechanical properties, which, in recent years, have made them candidates for protective coating materials on engineering components operating in extremely harsh and corrosive environments. These properties include high melting point, hardness, and stiffness combined with good corrosion, wear and thermal shock resistance. For a ceramic to act as a stable coating material, it should strongly adhere to the metal/alloy substrate, i.e., the bonding at the interface and the nature of electronic properties across the interface are of fundamental importance. We report predictions of the structural and bonding properties of interfaces formed between surfaces of iron and transition metal carbides and nitrides. Thermodynamic and mechanical considerations have restricted the choice of possible ceramics to only TiC, ZrC and BN. Ultrasoft pseudopotential plane-wave-based density functional theory (DFT) calculations, as incorporated in 'Vienna Ab-initio Simulation Package' (VASP) were performed using both the local density (LDA) and the generalized gradient approximations (GGA) for the exchange-correlation potential. A periodic 'supercell' or 'slab-model' approach was used to model the surfaces of iron and ceramics and the interfaces formed between them. Starting from calculations of the structural, cohesive and electronic properties of bulk Fe(bcc), Fe(fcc), TiC, ZrC, c-BN and h-BN and their several low-index ((100) , (110) and (111)) surfaces [1], we have constructed three interfaces having the lowest lattice mismatch between the Fe and the ceramic surfaces. These interfaces are the ones formed between (a) bcc-Fe(110) and c-BN(110) surfaces, (b) bcc-Fe(110) and ZrC(100) surfaces, and (c) fcc-Fe(111) and TiC(100) surfaces, having lattice mismatch of 0.1%, 1.2% and 2.2%, respectively. This talk will focus on the changes in the structural and electronic properties of iron and ceramics going from bulk to surfaces and finally to interfaces in terms of densities of states (DOS), charge transfer effects, relative stability, energy-level shifts, and relaxations and reconstructions. Our calculational results on bulk structures agree quite well with several other experimental and theoretical studies. We will also compare our predictions with previous predictions on TiC(100) surfaces and Fe-TiC interfaces, as well as photoelectron spectroscopic results on ceramic surfaces.

A. Arya and E.A. Carter, "First-principles studies of electronic and structural properties of TiC, ZrC and BN Surfaces" (to be submitted).

11:15 AM W3.12

LARGE-SCALE AB INITIO SIMULATIONS OF Fe-DOPED SrTiO₃ PEROVSKITES. R.A. Evarestov, Dept. of Quantum Chemistry, St. Petersburg University, St. Peterhof, RUSSIA; R.I. Eglitis, S. Piskunov, University of Osnabrueck, Dept. of Physics, Osnabrueck, GERMANY; E.A. Kotomin, Institute of Solid State Physics, University of Latvia, Riga, LATVIA and Max Planck Institut für Festkörperforschung, Stuttgart, GERMANY; G. Borstel, University of Osnabrueck, Dept. of Physics, Osnabrueck, GERMANY.

Using the Unrestricted Hartree-Fock method and supercells containing up to 160 atoms, we calculated the energy level positions in the gap and atomic geometry for the Fe⁴⁺ impurity substituting for a host Ti atom in SrTiO₃. In agreement with experiment, the high spin (S=2) state is much lower in energy than the zero-spin state. The energy level positions strongly depend on the asymmetric displacement mode of the six nearest O ions which is a combination of the Jahn-Teller and breathing modes. A considerable covalent bonding between the Fe ion and four nearest O ions takes place. Results are compared with available experimental data.

11:30 AM W3.13

MOLECULAR DYNAMICS STUDIES OF THE KINETICS OF PHASE CHANGES IN CLUSTERS II: CRYSTAL NUCLEATION FROM MOLTEN (RbCl)₂₅₆ AND (RbCl)₅₀₀ CLUSTERS.

Meihua Ma, Wenqing Lu, Department of Chemistry, Nanjing Xiaozhuang College, PR CHINA; Jinfan Huang, Department of Chemistry, University of Michigan, MI.

Molecular dynamics computer simulations have been carried out to study the effects of cluster size and the temperature on the nucleation rate of rubidium chloride clusters in the temperature range of 500K to 650K. Clusters with 256 and 500 RbCl molecules have been studied and the results are compared with those obtained from 108 molecule clusters. The melting point of the clusters were observed to increase with the size of the molecules in the clusters. The nucleation rate is found to decrease with increasing the cluster size or raising the nucleation temperature. Both classical nucleation theory and diffuse interface theory are used to interpret our observed results. Temperature dependence of interfacial free energy between the liquid and the solid is discussed.

11:45 AM W3.14

KINETIC MONTE CARLO SIMULATIONS OF STRAIN-INDUCED NANOPATTERNING OF HEXAGONAL SURFACES. M.L. Larsson, B. Lee, K. Cho, W. Nix, and B.M. Clemens, Stanford University, Dept. of Materials Science and Engineering, Stanford, CA.

Guided self assembly of periodic arrays of quantum dots has recently emerged as an important research field not only to reduce component size and manufacturing cost but also to explore and apply quantum mechanical effects in novel nanodevices. The intention of this kinetic Monte Carlo simulation study is to investigate self-organized nanopatterning of hexagonal surfaces for different periodic surface strain energies. The KMC model is a full diffusion bond-counting model including nearest neighbor as well as second-nearest neighbor interactions with an event catalogue consisting of 836 events modeling the effect of the strain modified surface energy. The surface strain energy in this study is caused by a hexagonal network of either dislocations or point defects at the interface between a substrate and a mismatched epitaxial layer of variable thickness. How the self organization is influenced by these different interfaces will be addressed. By changing the sign of the surface strain either a periodic array of quantum dots or a percolating network of quantum wires can be obtained, as a result of the deposited adatom kinetics, which suggests novel applications in quantum nanoelectronics, photonics and sensors.

SESSION W4: MULTISCALE AND MULTIPHYSICS SIMULATIONS

Chair: Antonios Zavaliangos
Wednesday Afternoon, April 3, 2002
Golden Gate C2/C3 (Marriott)

1:30 PM W4.1

A MULTISCALE ELASTIC MODEL FOR HETEROSTRUCTURE GROWTH. Geoffrey Simms, Mark Gyure, HRL Laboratories, LLC., Malibu, CA; Cameron Connell, Russel Cafilisch, UCLA Dept. of Applied Mathematics, Los Angeles, CA.

Elastic energy effects can manifest themselves visibly in the surface and interface structure or roughness of epitaxially grown semiconductors. The source of such elastic effects is a combination of intrinsic surface stresses and bulk elastic deformations. In particular, bulk deformation can be caused by the misfit strain associated with heterostructure assembly, and its effect on the growth kinetics at the surface determines the quality of subsequently stacked heterostructure interfaces. A model capable of computing the relevant features in the growth of semiconductor heterostructures must be able to efficiently solve elastic equations from the length scale of the atoms at the interface up to the scale of the heterolayers themselves. A multiscale model in the spirit of quasicontinuum methods is presented which, for the elastic solver, uses a valence force field energy at the atomistic scale and smoothly interfaces with larger patches in compositionally homogeneous regions. Growth kinetics are introduced by coupling with a continuous adatom field. Applications to the issues of step bunching and island ordering are addressed.

1:45 PM *W4.2

MULTISCALE COMPUTATIONAL MODELING OF NONLINEAR MATERIALS BEHAVIOR. Robert M. McMeeking, Department of Mechanical and Environmental Engineering and Materials Department University of California, Santa Barbara, CA.

Computational modeling in a multiscale approach will be described for a number of problems in materials nonlinear behavior drawn from ferroelectric switching, powder consolidation and the deformation of textile reinforced composite materials. In each of these problems, phenomena occur at a microscopic scale that influence the nonlinear response of the material. However, the resulting macroscopic response depends on the interaction of many microscopic units undergoing the phenomena. Therefore, an effective computational model must be capable of spanning the relevant length scales. For example, in the switching of a polycrystalline ferroelectric ceramic, the motion of the domain walls at the microscopic level leads to the switching behavior, but the shape of hysteresis loops results from the behavior averaged over many individual single crystals. Multiscale computational models will be described that recognize the effect of the motion of domain walls in individual crystals in the polycrystalline aggregate but that also predict the behavior of the aggregate over length scales encompassing many grains. Similarly, in powder consolidation, inelastic interactions among the individual powder particles are fundamental to the nonlinear behavior of the aggregate, but the overall aggregate behavior depends on the interactions among many hundreds of particles. Textile reinforced composite materials provide another example in which the behavior at the fiber and tow level is the basic nonlinear feature of the response due to fiber failure and

debonding. However, the macroscopic overall behavior of the composite material involves events occurring on a length scale encompassing many repeating unit cells of the textile pattern. Such problems provide interesting challenges in multiscale computational modeling.

2:15 PM W4.3

MULTISCALE MODELING OF THE DEVELOPMENT OF 3-DIMENSIONAL GRAIN STRUCTURES. Max Bloomfield, David Richards, Vinay Prasad, Ottmar Klaas, Dibyendu Datta, Mark Shephard, and Timothy Cale; Focus Center-New York, Rensselaer Polytechnic Institute, Troy, NY.

We have created a finite-element based, multiple level-set code to model the evolution and coalescence of islands during thin film growth. Grain boundaries are represented implicitly by a set of $N + 1$ scalar fields, $\phi_i(r, t)$ expressed on an unstructured mesh, subject to the condition that $\phi_i(r, t) = 0$ for all r on the boundary of grain i at time t [1]. Because each grain is associated with its own scalar field, properties can be easily retained on a grain-by-grain basis. The time evolution of each grain is computed separately using the level set equation [1] based upon surface velocities computed from a user-specifiable model. Level sets representing different regions are reconciled to bring them into agreement. We have developed a novel contour extractor to define interfaces uniquely and robustly. We use a "redistancing" algorithm [2] to address motion-induced and reconciliation-induced distortions in the scalar field associated with each grain. This step stabilizes the evolution, allowing for simulations that include the coalescence of proto-grains and islands into complex grain structures. Demonstrations of this code are presented, including the use of the grain scale code in a multiscale simulation framework. Reactor scale simulations of reactant transport are performed using a FEM code. Reactant data are passed from the grain scale to this scale as boundary conditions. This allows us to establish concentration fields of reactant both on the scale of $0.1\mu m$, and using local refinement, on the $0.1mm$ scale. The reactor-scale simulation passes reactant data back down to a grain-scale level set simulation. This allows us to show the interaction of phenomena such as reactor-scale reactant depletion on the resulting grain structure.

1. S. Osher and J.A. Sethian, J. Comp. Phys. 79, 12 (1988).
2. T.J. Barth and J.A. Sethian, J. Comp. Phys. 145, 1 (1998).

2:30 PM W4.4

DYNAMICS OF A NON HOMOGENEOUSLY COARSE GRAINED SYSTEM. Stefano Curtarolo, Gerbrand Ceder, Dept of Material Science and Engineering, MIT, Cambridge, MA.

A key issue in materials modeling is to study systems simultaneously at all the length scales where the important physics for a particular property takes place. A systematic approach to such models requires a description in which matter can be coarse grained to arbitrary levels, are necessary. Attempts to do this in the static regime (i.e. zero temperature) have already been developed. In this work, we show an approach that leads to a dynamics for such coarse-grained models. This allows us to obtain temperature-dependent and transport properties. Renormalization group theory is used to create new local potentials model between nodes, within the approximation of local thermodynamical equilibrium. Assuming that these potentials give an averaged description of node dynamics, we calculate thermal and mechanical properties. If this method can be sufficiently generalized it may form the basis of a Molecular Dynamics method with time and spatial coarse-graining.

3:15 PM W4.5

THE ROLE OF THE ATOMISTIC SIMULATION IN A MULTISCALE APPROACH FOR MODELING PLASTICITY IN CRYSTALLINE SOLIDS. Guofeng Wang, Alejandro Strachan, Tahir Cagin, William A. Goddard III, Materials and Process Simulation Center, Caltech, Pasadena, CA.

At finite temperatures, the motion of the $1/2a \langle 111 \rangle$ screw dislocation in bcc metal consists of two steps: kink pair nucleation and subsequent lateral motion of the component kinks. Using molecular dynamics (MD) simulations with the qEAM force field, we studied the multiplicity, formation energy, lateral motion energy barrier, and structural features of $1/3a \langle 112 \rangle$ kinks in the $1/2a \langle 111 \rangle$ screw dislocation in Tantalum (Ta). We find two, energy degenerate, three fold symmetric cores for the $1/2a \langle 111 \rangle$ screw dislocation (denoted as P and N) lead to 2 kinds of the flips (denoted as P-N and N-P), 8 kinds of the isolated kinks and 16 combinations of the kink pairs. The lowest formation energy for each kind of dislocation defects is 0.005 eV of flip P-N, 0.139 eV of isolated kink PLN and 0.794 eV of kink pair PLN-NRP. We estimate the energy barrier to be 3.5×10^{-4} eV and 2.5×10^{-4} eV for PLN and NRP kink for lateral motion, respectively. A detailed structural analysis of kink shows that NRP is the elementary right kink and PLN is the basic left kink (the others are the composites of the elementary kinks and flips). Therefore, the

kink pair PLN-NRP has the lowest nucleation energy (0.794 eV) and the highest lateral motion mobility among all possible kink pairs. The information obtained from atomistic simulations was passed into a kink pair mechanism based macroscopic model. The resulting atomistically informed model captures the main features in the empirical temperature dependence of stress-strain curves and strain rate dependence of stress-strain curves.

3:30 PM W4.6

MECHANISTIC TUNING OF RATE EQUATION MODELS FOR AGGREGATION USING LARGE-SCALE MOLECULAR DYNAMICS. Manish Prasad and Talid Sinno, Department of Chemical Engineering, University of Pennsylvania, Philadelphia, PA.

Solid-state nucleation and aggregation are ubiquitous in materials processing and a mechanistically accurate description of these processes is imperative for modeling of process/property relationships. An inherent challenge in such problems is the multi-scale nature of aggregation in which single atoms aggregate to form structures that can be as large as microns and beyond. Furthermore, the process description ultimately often must be on the continuum scale for direct comparison to experiment. A multi-faceted approach for investigating aggregation in crystalline materials is presented using the example of vacancy aggregation in silicon. The essential ingredient in this framework is a direct, quantitative comparison between the predictions of continuum and atomistic simulations for the transient size distribution of vacancy clusters. The empirical Environment-Dependent Interatomic Potential (EDIP) is used first to develop a comprehensive thermodynamic picture for individual vacancy clusters. Next, a highly efficient parallel molecular dynamics code is used to simulate the dynamical evolution of vacancy clusters in a system of 1000 vacancies dispersed in a host lattice containing 216,000 Si atoms. The simulation spans several nanoseconds of real time, which is sufficient to capture the initial stages of void nucleation in a statistically meaningful manner. This data is used to investigate mechanistically a mean-field approximation for the identical process in which all thermophysical property input is provided internally consistently from EDIP atomistic simulations. Quantitative comparison between the two representations leads to a very accurate rate-equation model for vacancy aggregation at short time and length scales. The mean-field model subsequently is extended to macroscopic length and time scales and compared directly to experimental data for void formation in silicon. It is shown that this approach leads to significantly improved models for vacancy aggregation. The improvements are due to previously excluded diffusion mechanisms and more rigorous expressions for the aggregation and dissolution rates.

3:45 PM W4.7

MULTISCALE MODELING OF WAVE PROPAGATION: FDTD/MD HYBRID METHOD. Krishna Muralidharan, P. Deymier and J.H. Simmons, Dept of MS&E, University of Arizona, Tucson, AZ.

Atomic level processes often play an important role in the way a material responds to an external field. Thus in order to model the behavior of materials accurately, it is necessary to develop simulation techniques which can effectively couple atomistic effects to the macroscopic properties of the model system and vice-versa. In other words, a multiscale methodology needs to be developed to bridge the different length and time scales. In this work we study the propagation of an elastic wave through a medium in which the composition and the density are functions of the stress. The equations of motion for the wave propagation through the continuum are solved using the Finite Difference Time Domain Method (FDTD). Simultaneously we use Molecular Dynamics (MD) to examine the effect of this periodic field on the atomic dynamics and the effect of atomic dynamics on the propagation of the wave. The handshaking between the FDTD region and the MD region is concurrent and achieved by imposing appropriate boundary conditions. This material is based upon work supported by the National Science Foundation under Grant No. 9980015.

4:00 PM W4.8

DAMAGE MECHANISMS OF FILLED SILOXANES FOR PREDICTIVE MULTISCALE MODELING OF AGING BEHAVIOR. Bryan Balazs, Robert Maxwell, Steve deTeresa, Long Dinh, Rick Gee, Lawrence Livermore National Laboratory, Livermore, CA.

Predictions of component performance versus lifetime are often risky for complex materials in which there may be many underlying aging or degradation mechanisms. In order to develop more accurate predictive models for silica-filled siloxane components, we are studying damage mechanisms over a broad range of size domains, linked together through several modeling efforts. Atomistic and molecular dynamic modeling has elucidated the chemistry of the silica filler to polymer interaction, as this interaction plays a key role in this materials aging behavior. This modeling work has been supported by

experimental data on the removal of water from the silica surface, the effect of the surrounding polymer on this desiccation, and on the subsequent change in the mechanical properties of the system. Solid State NMR efforts have characterized the evolution of the polymer and filler dynamics as the material is damaged through irradiation or desiccation. These damage signatures have been confirmed by direct measurements of changes in polymer crosslink density and filler interaction as measured by solvent swelling, and by mechanical property tests. Data from the changes at these molecular levels are simultaneously feeding the development of age-aware constitutive models for polymer behavior. In addition, the microstructure of the foam, including under load, has been determined by Computed Tomography, and this data is being introduced into Finite Element Analysis codes to allow component level models. All of these techniques are directed towards the incorporation of molecular and microstructural aging signatures into predictive models for overall component performance.

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 # W-7405-ENG-48.

SESSION W5: POSTER SESSION

Chair: Veena Tikare

Wednesday Evening, April 3, 2002

8:00 PM

Salon 1-7 (Marriott)

W5.1

STEP BUNCHING CAUSED BY ENERGY BARRIERS AT STEPS. S.Y. Leung, M.H. Xie, Department of Physics, The University of Hong Kong, Hong Kong, HONG KONG; S.Y. Tong, Department of Physics and Material Science, City University of Hong Kong, Kowloon, HONG KONG.

It is known that an asymmetry for adatoms incorporation at steps results in specific morphology of the surface. For example, on a vicinal surface, the presence of a (positive) Ehrlich-Schwoebel (ES) barrier causes steps to grow predominantly by adatom capture from terraces below, which in turn leads to uniform terrace width. On the other hand, if the kinetics favors adatom incorporation from upper terraces, step bunching will occur. Obviously, both negative ES barrier that promotes adatoms to easily diffuse down a step; and positive incorporation barrier impeding adatoms captured by the ascending step, have the similar effect that leads to step growth to be dominated by adatoms on upper terraces. This study shows, however, that only the positive incorporation barrier accounts for the step bunching. The analytical prediction is confirmed by kinetic Monte Carlo simulations.

W5.2

THEORETICAL AND EXPERIMENTAL INVESTIGATION OF THERMAL STABILITY OF HfO₂/Si AND HfO₂/SiO₂ INTERFACES. Chun-Li Liu, Matt Stoker, Rama I. Hegde, Raghav S. Rai, and Philip J. Tobin, Advanced Process Development and External Research Laboratory, Motorola, Inc., Mesa, AZ.

The assessment of the thermal stability across HfO₂/Si and HfO₂/SiO₂ interfaces has been difficult due to lack of thermodynamic data. We present the results of thermodynamic calculations intended to fill this gap. A thermodynamic model was developed by assuming that HfSiO₄ is an ideal solution of HfO₂ and SiO₂ to a first order approximation. The theoretical results predict that the HfO₂/Si interface is thermodynamically stable up to 1100°C, while the HfO₂/SiO₂ interface is thermodynamically unstable even at room temperature. Our experimental results from TEM and XPS analysis are consistent with these modeling predictions.

W5.3

MOLECULAR DYNAMICS SIMULATION OF ASPERITY SHEAR IN ALUMINUM. Jun Zhong, James B. Adams, Arizona State University, Dept of Chemical and Materials Engineering, Tempe, AZ; Louis G. Hector, Jr., General Motor R&D Center, Materials and Processes Laboratory, Warren, MI.

One important wear mechanism involves the shear of asperities by other asperities. We use molecular dynamics to simulate the shearing of aluminum asperities by a "hard" (Lennard-Jones) asperity. These simulations involve the use of a reliable EAM potential for Al that was developed by Force Matching Method to a large database of DFT forces. The simulations are repeated for a wide range of conditions, including asperity drift velocities, temperatures, asperity shapes, degree of intersection, crystal orientations and adhesive strengths, to determine their effect on the wear process. The thermal effects, mechanisms of deformation on Al substrate during asperity shear are also discussed.

W5.4

TIME DEPENDENCE OF THE SEGREGATION OF DIFFUSING SOLUTE IN POLYCRYSTALLINE MATERIAL. Irina V. Belova and Graeme E. Murch, Diffusion in Solids Group, University of Newcastle, NSW, AUSTRALIA.

At long times, the partitioning of diffusing solute between grains and grain boundaries is governed by an equilibrium equation. At short times however the diffusing solute from a source cannot sample enough grains and grain boundaries to establish such an equilibrium, although this is the usual tacit assumption. In this computer simulation study we employ a grid method to study the time dependence of solute partitioning for diffusion from a thin-film solute source. It is shown that at short times the solute follows a partitioning equation indicative of infinite grains and grain boundaries. At longer times, as the solute is able to sample more of the actual nature of the environment, the partitioning equation changes to one indicative of a finite system.

W5.5

ESTIMATION OF THE PHENOMENOLOGICAL EFFECTIVE DIFFUSIVITY IN NANOCRYSTALLINE MATERIALS.

Irina V Belova and Graeme E. Murch, Diffusion in Solids Group, University of Newcastle, NSW, AUSTRALIA.

The Hart equation has long provided the means for estimating the effective phenomenological diffusivity of a diffusant migrating in a polycrystalline material. However, for nanocrystalline materials, where a large fraction of atoms reside in grain boundaries, assumptions in the derivation of the Hart equation make it unlikely that it provides an adequate description. The Maxwell-Garnett equation used for describing the effective diffusivity in porous media has recently been extended by Kotomin and co-workers to quite general conditions. In the present paper, computer simulation of a fine-grained grid model is used to test the Hart and Maxwell-Garnett equations for various random and ordered packed arrangements of cubes and spheres. It is shown that the extended Maxwell-Garnett equation is greatly superior to the Hart equation and should provide a satisfactory description of the effective diffusivity in nanocrystalline materials.

W5.6

A FULL POTENTIAL DFT STUDY OF SINGLE-WALL NANOTUBES AND THE EFFECTS OF INTERTUBE COUPLING.

X. Duan, Computer Science Corporation, ASC MSRC, Wright-Patterson AFB, OH; B. Akdim, Z. Wang, R. Pachter, and W.W. Adams, Air Force Research Laboratory, Materials & Manufacturing Directorate, AFRL/MLPJ, Wright-Patterson AFB, OH.

We present a full potential linear combination of atomic orbitals (FP-LCAO) density functional theory study of the structural, mechanical, electronic, and optical properties of selected nanotube systems. This accurate all-electron scheme was applied so far by Matie [1], who studied the electronic properties of a bent isolated large carbon nanotube molecule. The FP-LCAO results are compared to other calculations, such as the pseudopotential LCAO, tight-binding, and empirical approaches. In addition, a comparative study between the properties of a crystalline-rope and isolated tubules is to be discussed, which highlights the effects of intertube coupling due to Van der Waals interactions.

[1]- A. Matie, Chem. Phys. Lett., 331, 21 (2000).

W5.7

MICROMAGNETICS SIMULATION ON ASYMMETRIC PSEUDO-SPIN VALVE DOTS. NgocNga Dao and Scott L.

Whittenburg, University of New Orleans, Department of Chemistry/AMRI, New Orleans, LA; Fernando Castano and Caroline A. Ross, Massachusetts Institute of Technology, Department of Materials Science and Engineering, Cambridge, MA.

We present our recent simulated results for $\text{Ni}_{79}\text{Fe}_{21}/\text{Cu}$ (t nm)/Co (4nm) pseudo-spin valves. The spacer, t, has two thicknesses: 3 nm and 6 nm. We have simulated two rectangular dot sizes, 70 nm x 180 nm and 70 nm x 550 nm for these films. Our simulations show a reasonable agreement with the experimental results. A fast switching between two magnetic layers is observed. We will also present the magnetic domain structures resulting from these calculations

W5.8

FROM BIFURCATIONIS TO CHUA'S PERIODIC TABLE.

Roberto Tonelli, Franco Meloni, INFN-Phys. Dept. University of Cagliari, ITALY; L.O. Chua, ERL-University of California, Berkeley, CA.

We describe and discuss the similarity in the behaviour of two different kind of physical systems: Chua's Circuit (and more in general chaotic systems) and atoms in the Periodic Table. We analyze

the regularities arising from the chaotic nature of the former against the regularity in the energy spectra of the seconds. We show the similarities among the Bohr's law and the bifurcation diagram building a map connecting each energy level in atoms to each point in the bifurcation diagram in the parameter space. We found a general rule valid for many elements of the Periodic Table by calculating two-dimensional bifurcation diagram versus Bohr's law. The result is a one-to-one correspondence between atoms and nonlinear Chua's circuits. Finally we discuss possible implications of the model when applied to more complicated systems like molecules or atomic clusters.

W5.9

BASE-CATALYTIC PROPERTIES OF SOLID SILICON IMIDONITRIDES. Peter Kroll, Institute of Inorganic Chemistry, RWTH Aachen, GERMANY.

Polymer-derived silicon imidonitride solids are studied using density functional methods. Key properties of this new material class are the pore size distribution, which can be designed to peak sharply (e.g. at 5-7 Å), and the capability to selectively catalyze reactions in the micro-porous amorphous solids. We generated atomistic models of silicon imidonitride using amorphous silicon nitride structures and carving suitable pores in them. The two model systems with Si-N and N-H bonds only we consider have pore sizes of 4.5 Å and 6 Å, respectively, with a minimum thickness of the surrounding framework of 5 Å. N-H and N-H₂ groups are located at the internal surfaces, generating a basic environment within the pores as indicated by the high electron density. Calculated Raman spectra compare very well with experimental results. We studied the hydrogen mobility at the internal surfaces by Car-Parrinello molecular dynamic simulations. Protons diffuse more rapidly than in bulk materials and the migration occurs through interaction with adjacent N atoms. We studied the base-catalytic properties by inserting benzaldehyde and malononitrile into the model and investigating the reaction path of a Knoevenagel coupling reaction.

W5.10

MESOMECHANICAL INVESTIGATION OF THE EFFECT OF MICROSTRUCTURES OF MATERIALS REINFORCED WITH BRITTLE PARTICLES ON THE FRACTURE RESISTANCE AND FRACTALITY OF FRACTURE. L. Mishnaevsky, Jr., U. Weber, S. Schmauder, University of Stuttgart, State Materials Testing Institute(MPA), Stuttgart, GERMANY.

This paper seeks to study systematically the effect of microstructures of materials reinforced with brittle hard particles on their fracture behavior and toughness. Using the computational experiment approach [1], the authors studied different arrangements of brittle inclusions and simulated the crack growth and fracture resistance in the microstructures (high speed steels). The following arrangement of brittle inclusions in the materials were considered: net-like continuous, band-like, random with different inclusion sizes, gradient and clustered arrangements, with different inclusion sizes and orientations. Crack paths for each of the microstructures were simulated. The force-displacement curves were determined numerically. The fracture toughness and the fractal dimension of fracture surfaces are determined numerically for each microstructure. Main mechanisms of the toughening effect of the complex microstructures are identified: crack path deviation from its initial direction, and large areas of tough matrix between the areas of high inclusion density. It is shown that a very high fracture toughness of materials can be achieved if a growing crack can be forced to follow the brittle inclusion network. Yet, such a mechanism of toughening is shown to be unstable: if the crack stops to follow the network and propagates through the bands, the toughness drops drastically. It is demonstrated that extensive crack deviations from the initial cracking directions and the increase in the fracture toughness can be most efficiently achieved by using complex microstructures, like alternated layers of fine and coarse inclusions.

References:

1. L. Mishnaevsky Jr, M. Dong, S. Hoenle and S. Schmauder, Computational Mesomechanics of Particle-Reinforced Composites, Comp. Mater. Sci., Vol. 16, 1999, No. 1-4, pp. 133-143 2. L. Mishnaevsky Jr and S. Schmauder, Continuum Mesomechanical Finite Element Modeling in Materials Development: a State-of-the-Art Review, Applied Mechanics Reviews, Vol. 54, 1, 2001, pp. 49-69.

W5.11

DEVELOPMENT OF THEORETICAL MODEL FOR CALCULATING THE LATTICE THERMAL CONDUCTIVITY IN GALLIUM NITRIDE AND RELATED COMPOUNDS.

Dmitri Kotchetkov, Jie Zou and Alexander Balandin, Dept of Electrical Engineering, Univ of California, Riverside, CA.

We report on the development of a theoretical model for calculating the lattice thermal conductivity in GaN and related compounds. The model is based on the solution of Boltzmann's transport equation and accurate account of acoustic phonon relaxation mechanisms,

characteristic for a given material system. In particular, we consider the following thermal resistive processes: (i) three-phonon Umklapp scattering due to crystal anharmonicity; (ii) scattering of phonons on impurities and point defects; (iii) scattering of phonons on short-range (core) and long-range (screw and edge) fields of threading dislocations. Mass and volume differences of impurity atoms are taken into account to achieve accurate results. The first round of simulation runs allows us to determine correctness of values of the basic material parameters of GaN, such as Debye temperature and elastic constants extracted from different sets of experimental data. In addition, the best algorithm for sound velocity calculation is determined. The second round of simulation results in accurate estimate of specific impurity concentrations, the values of dislocation line density and mutual orientation of the temperature gradient and dislocation lines. During the second round of simulation different possible combinations of major impurities (H,O,C) and Si doping concentrations of n-type GaN are studied. Knowing the thermal conductivity of GaN sample, one can use our model to estimate dislocation line density and impurity concentrations in GaN sample. On other hand, if density of dislocations and defects are known, one can accurately predict the value of thermal conductivity. The latter is important, since GaN and related compounds typically have very large concentrations of defects [1].

[1] D. Kotchetkov, A. Balandin, (Mat. Res. Soc. Symp. Proc. Vol. 680E).

W5.12

Abstract Withdrawn.

W5.13

THE DESCRIPTION OF LOW-SYMMETRICAL METALLIC CRYSTALS STABILITY, ACCOUNTING A NON-CENTRAL INTERATOMIC INTERACTIONS. Mikhail A. Baranov, Evgenya V. Chernyh, Veronika V. Romanenko, Mikhail D. Starostenkov, General Physics Dept, Altai State Technical University, Barnaul, RUSSIA.

The interatomic potentials, described the atomic interactions in HCP metals Ti, Co, Cd, Mg, Zn, Hf and in alloys Ti_3Al , Mg_3Cd are presented by Morse function. It is modulated function, which depends on the direction of the bond vector in the crystal. The corresponding equipotential surfaces are situated near spherical ones only at very small or big values of r . That is why the force lines of this potentials differ essentially from the radial straight lines. This circumstance testifies to the non-central nature of the interatomic interaction. The stability of crystal is achieved at experimental values of the elementary cell sizes, energy of sublimation and the bulk module. The values of the heat of HCP/FCC phase transformation in metals and heat of order-disorder phase transformation in alloys are corresponded to experimental data. The energetical and configuration characteristics of the wide class of planar and point defects are sufficiently described in the frames of this model.

W5.14

A FIRST PRINCIPLE EXPLANATION OF INITIAL GROWTH RATE OF SiO_2 . Shahriar Anwar, James B. Adams, Arizona State University, Chemical & Materials Engineering, Tempe, AZ.

The anomalous initial growth rate of thermally grown silicon dioxide has been the subject of much discussion since the publication of a monumental paper by B. Deal and A. Grove in 1965. Several empirical models have been proposed to explain this phenomenon, but none has received wide acceptance. We present a radically new explanation based on fundamental thermodynamical calculations that explains the phenomena without resorting to any empirical parameters.

W5.15

MATHEMATICAL MODELLING OF MICROSTRUCTURAL EVOLUTION DURING HOT ROLLING OF LOW CARBON BAINITIC STEELS. Andrzej Lis, Jadwiga Lis, Leopold Jezorski, Technical University of Czestochowa, Institute of Materials Engineering, Czestochowa, POLAND.

The constitutive equations for yield stress of ULCB-Mn and ULCB-Ni steels in a function of strain intensity, strain rate and temperature of hot deformation were established. New relationships describing softening and recrystallization kinetics of austenite during hot rolling of plates as well as bainitic ferrite grain size evolution when accelerated cooling was used, were applied for an effective control of thermomechanical processing in the industry to achieve required properties of final products. During the study of the influence of structural parameters of bainitic steels on: yield strength, impact strength, fracture toughness and impact transition temperature, it has been shown, that besides the former austenite grain size which existed before austenite to bainite ferrite transformation, the sizes of the lathes and packets of the bainite-martensite microstructures should be taken into account as those which determine the mean grain size of fracture facets in the function of the rates of accelerated cooling of

plates. The proposed mathematical model can be used for various kinds of applications such as: design of chemical composition and manufacturing conditions of steel, prediction of mechanical properties of products and process control to reduce scattering of properties.

W5.16

DIAGRAMS OF PHASES STABILITY FOR TWO-DIMENSIONAL SYSTEMS Ni-Al, Ni-Fe, Cu-Au. Mikhail D. Starostenkov, Gennadiy M. Poletayev, Julia V. Patzeva, General Physics Dept, Altai State Technical University, Barnaul, RUSSIA.

Diagrams of phases stability were made for two-dimensional systems at the temperatures near absolute zero in the limits of the model, where interatomic interactions were described with the help of Morse pair potentials. Diagrams contain the dependence graphs of specific configuration energy on concentration of components for all possible phases of binary systems. Different variants of two-dimensional crystal superstructures, disordered state and bimetals, containing both phases of pure components were studied. The spheres of minimum values of configuration energy were marked at the diagrams after applying of all the graphs. Phases, corresponding to the given spheres, were characterized as stable ones in the limits of the calculated area of component concentration. Melting temperatures were determined by the method of molecular dynamics for stable phases.

W5.17

COMPUTER SIMULATION STUDIES OF FRACTURE IN VITREOUS SILICA. Romulo Ochoa, Michael Arief, College of New Jersey, Dept. of Physics, Ewing, NJ; Joseph H. Simmons, University of Arizona, Dept. of Materials Science and Engineering, Tucson, AZ.

We present molecular dynamics computer simulations of fracture by modeling silica glass using the van Beest, Kramer, and van Santen potential (BKS). This model has the Born-Mayer-Huggins functional form with an additional dispersion term, included to better simulate the covalent nature of silica. The BKS interatomic potential has proven to represent very effectively the structural and thermodynamical properties of crystalline and amorphous silica. Simulation samples, containing more than 3000 atoms, were stressed by applying uniaxial strain. Strain is applied by uniformly scaling particle positions periodically along one of the cell directions while holding the lengths of the other two sides fixed. At the strain rates applied, particle motions are dominated by thermal vibrations that allow the strain to redistribute itself within the structure. Strain rates of .004 - .4/ps were used. Comparisons with previous fracture simulations of silica that used the Soules force function are presented. We find that in both models, stress is relieved by rotation of the $(SiO_4)^{-2}$ tetrahedrons, increasing Si-O-Si bonding angles, and only small changes in the tetrahedron dimensions and O-Si-O angles. Samples fail at about 20 - 25% strain, without any visual indication of fracturing occurring. As samples are strained, about 10% past their failure point, they fracture suddenly, with surfaces forming within a few picoseconds. When this occurs, the samples' densities increase to approximately their initial values. As the samples continue to be strained, any additional free space collects between the surfaces formed. We have analyzed the variations of local densities and void sizes (void coalescence), as function of strain (and time) and present our results as short color-coded movies.

W5.18

SIMULATION OF POLYCRYSTALLINE CERAMICS WITH MICRO-CRACKS. Jianwu Cao, Yoshihisa Sakaida, Yasuo Nagano and Hiroshi Kawamoto, Synergy Ceramics Laboratory, Fine Ceramics Research Association, Nagoya, JAPAN.

The micro FEM model, which was considered in the middle bottom of a four-point bending macro FEM model, was constructed from SEM micrograph of an Al_2O_3 -10vol% ZrO_2 ceramics, in which the crystallographic information was given to each grain randomly. One micro-crack was introduced in the micro FEM model as a basic case to simulate the four-point bending strength. The strength was determined by the average stress in a one grain size distance from the crack tip. Two types of micro-cracks were introduced in the model as a second micro-crack, and the strength were compared with the basic case. For the case that the second crack is parallel to the first crack and apart from the first crack in horizontal direction, the strength increasing with the second crack closer to the first crack. For the case that the second crack is parallel to the first crack and apart from the first crack in vertical direction, the strength decreasing with the second crack closer to the first crack.

W5.19

COUPLING OF ORBITAL FREE DENSITY FUNCTIONAL THEORY TO FINITE ELEMENT METHODS: "FIRST PRINCIPLES" STRESSES FOR MACROSCOPIC NANO-INDENTATION SYSTEMS. Robin L. Hayes, Emily A. Carter, UCLA, Dept. of Chemistry and Biochemistry, Los Angeles, CA; Matt

Fago, Michael Ortiz, Caltech, Dept. of Aeronautical Engineering, Pasadena, CA.

Finite Element Methods (FEM) can be used to predict deformation and phase transformations in micron-sized materials, but are limited by the accuracy of the underlying stress and energy calculations. Our implementation involves energy minimization within the framework of continuum mechanics, and requires the computation of energy density and its derivatives at discrete points in the finite element mesh. Currently, we treat each integration point within the Cauchy-Born approximation as a homogeneous deformation of a representative crystal lattice. The response of these "representative atoms" to the macroscopic deformation then provides the energy and stress tensor, and by relaxation with respect to the basis vectors can capture local deformations and phase transformations. Previously, empirical methods, rather than the more accurate, but computationally expensive, first principles methods, have been used, since each FEM simulation can require hundreds of thousands of stress calculations. Orbital Free Density Functional Theory (OFDFT) provides rapid, first principles evaluation of the energy and stress tensor. Unlike, Kohn-Sham DFT, only the density, not the orbitals are used, so the method scales linearly with the number of electrons. Although capable of handling > 1000 atoms, a macroscopic material with millions of atoms is beyond the reach of OFDFT. By linking OFDFT with FEM, we gain the best features of both: large length scales with first principles accuracy. Furthermore, each integration point can be calculated independently, so this method is highly amenable to parallelization. Results for nano-indentation of aluminum and its alloys will be discussed.

W5.20

A MODEL FOR COMPREHENSIVE STUDIES OF POROSITY IN MESOPOROUS LOW-K DIELECTRICS. Mihail P. Petkov, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA.

The successful integration of a low-dielectric-constant (low-k) material as an interlayer dielectric (ILD), as well as its resistance to a hostile (chemical, thermal, radiation, etc.) environment depends on the morphology of the embedded porosity. This is a preliminary comprehensive study based on a simple percolation model, which is applied to represent randomly packed non-interacting hard (non-overlapping) spheres (pores). Analysis of the number of connected and isolated pores is used to evaluate the pore connectivity at a given porosity below the onset for percolation. These results are related to some of the presently available ILD candidates for the 0.13 μm feature-size generation. The importance of the percolation threshold, at which an "infinite" pore cluster is formed, will be assessed in the light of the requirements given in the International Technology Roadmap for Semiconductors. The feasibility of the model for studying changes in material properties and the possibilities for future developments will be discussed.

SESSION W6: MICROSTRUCTURAL EVOLUTION I

Chair: Corbett Battaile
Thursday Morning, April 4, 2002
Golden Gate C2/C3 (Marriott)

8:00 AM *W6.1

PHASE-FIELD STUDY OF THE CELL-DENDRITE TRANSITION IN DIRECTIONAL SOLIDIFICATION OF DILUTE BINARY ALLOYS. Blas Echebarria and Alain Karma, Dept. of Physics and Center for Interdisciplinary Research on Complex Systems, Northeastern University, Boston, MA.

Despite several decades of theoretical study of directional solidification after the pioneering analysis of Mullins and Sekerka on morphological stability, several fundamental aspects of the formation of cellular and dendritic array structures remain poorly understood. We present results of a numerical study of these array structures that is based on a new phase-field formulation of the solidification of dilute binary alloys [A. Karma, Phys. Rev. Lett, Vol 87, 115701 (2001)]. This formulation enables us to simulate quantitatively microstructural pattern formation in the limit where the solid-liquid interface is close to thermodynamic equilibrium (i.e. with negligible interface kinetics and solute trapping), and hence to establish direct quantitative comparisons with existing low velocity benchmark data in transparent organic and metal systems. The simulation results shed light on the origin of the morphological instability that underlies the cell to dendrite transition and on the crucial roles of crystalline anisotropy and thermal noise.

8:30 AM W6.2

EFFECT OF COALESCENCE ENERGY RELEASE ON THE SHAPE EVOLUTION OF NANOPARTICLES AND THE ONSET

OF AGGREGATE FORMATION. D. Mukherjee, University of Minnesota, Minneapolis, MN; K.E.J. Lehtinen, University of Helsinki, FINLAND; and M.R. Zachariah, University of Minnesota, Minneapolis, MN.

The driving force for coalescence of two nanoparticles is the reduction in free energy through a reduction in surface area. The resulting particle also has a lower total potential energy, which through conservation of energy can lead to a significant increase in particle temperature. In a vapor-condensation growth process the coalescence energy release competes with heat transfer and if heat loss is small significant enhancements to the primary particle size may be observed. In this paper we develop a model that illustrates that this heat increase can be extremely important and should be accounted for when modeling collision/coalescence processes. The calculation methodology involves combining classical molecular dynamics methods for property determination and a kinetic monte carlo approach to simulate, the ensemble aerosol, coagulation, sintering and non-isothermal effects associated with coalescence generated heat release. Our calculations indicate that the heat release associated with particle coalescence may reduce the coalescence time by as much as a few orders of magnitude. It is shown that accounting for energy release and heat transfer effects have a dramatic effect on primary particle formation and the onset of aggregate formation. We also show that a simple coalescence model, which includes the temperature effect, closely follows our prior molecular dynamics calculations for silicon nanoparticle sintering. This analysis also explains a set of experimental results for alumina nanoparticle production, previously unexplainable by classical methods.

8:45 AM W6.3

RIETVELD REFINEMENT FOR QUANTITATIVE TEXTURE AND STRAIN EVOLUTION DURING STRESS-INDUCED TRANSFORMATIONS IN SHAPE-MEMORY ALLOYS. Raj Vaidyanathan, University of Central Florida, AMPAC/MMAE, Orlando, FL; Mark A.M. Bourke, Los Alamos National Laboratory, Los Alamos, NM; David C. Dunand, Northwestern University, Department of Materials Science and Engineering, Evanston, IL.

The stress-induced transformation of nickel-rich NiTi from a cubic phase to a monoclinic phase can result in tensile strains as high as 8% under applied stress. On unloading, the monoclinic phase becomes unstable and transforms back to the parent phase, with a concomitant macroscopic strain recovery. By recording neutron diffraction spectra during mechanical loading, such reversible stress-induced transformations can be investigated as they occur. A Rietveld refinement methodology is established for quantitative texture and strain determination from such data during stress-induced phase transformations. Two formulations of the elastic strain from the refinement procedure are described. In the first approach, the refinement incorporates no description of any strain anisotropy and the strain is determined from lattice parameters obtained as best fits. In the second approach, a strain anisotropy term is incorporated in the Rietveld procedure and the strain is reported for a specific crystallographic plane as a contribution of isotropic (hkl-independent) and anisotropic (hkl-dependent) components. Two differing approaches for the texture evolution are used. In the first, a cylindrical symmetrical version of an ellipsoidal model is used to describe the texture. In the second, a generalized spherical-harmonic description of the orientation distribution function (which maps the probability of each of the possible grain orientations with respect to the external sample dimensions) is used.

9:00 AM W6.4

SIMULATION OF MICROSTRUCTURAL EVOLUTION DURING THERMOMECHANICAL CYCLING IN Pb-Sn SOLDERS. Michael W. Woodmansee, Veena Tikare, Sandia National Laboratories, Albuquerque, NM.

Solder joints in electronic interconnects are subject to thermo-mechanical cyclic fatigue due to thermal expansion mismatch of the joined components. Solder joints subjected to such fatigue develop bands of coarsened microstructure and eventually fail catastrophically in these coarsened bands. We will present a model that is capable of simulating the stress-induced coarsening in Pb-Sn solders. This model is a kinetic, Monte Carlo model which can simulate coarsening coupled to a finite element model called OOF which simulates the mechanical state of a microstructure under different loading conditions. The microstructural evolution due to coarsening of grains by curvature driven grain growth and of phase coarsening by long range diffusion is simulated by the Monte Carlo model. The mechanical state of the microstructure in response to the thermomechanical loading is calculated by OOF. This stress state is then used by the Monte Carlo model to simulate further microstructural evolution under the applied stress. The results of this model will be presented. The capabilities and limitations of this model will be discussed.

9:15 AM *W6.5

STRESS EFFECTS ON MICROSTRUCTURAL EVOLUTION IN TEXTURED POLYCRYSTALS. Elizabeth A. Holm, Corbett C. Battaile, Materials and Process Modeling Department, Sandia National Laboratories, Albuquerque, NM; William A. Counts, Materials Science and Engineering Department, Georgia Institute of Technology, Atlanta, GA.

In engineered materials from polycrystalline thin films to forged alloys, internal stresses govern microstructural evolution. In this study, we couple a mesoscale polycrystal plasticity finite element model for stress development with discrete and continuum models for grain growth to elucidate the interdependence of microstructural evolution and mechanical state. Because we find that grain orientation is the primary factor in determining local stress levels, texture is critical to the macro- and mesoscopic mechanical response of a microstructure, as well as to its evolution. We observe and characterize the formation of load-bearing networks of grains as a function of texture, and we correlate internal stress with grain characteristics such as size, shape, etc. Of particular interest are stress concentrations where damage (i.e. cracks, voids) may initiate in the microstructure. Finally, just as mechanical state influences evolution, so too does grain growth alter the internal stress distribution. In a series of iteratively coupled grain growth and plasticity simulations, we model stress-assisted grain growth during tensile deformation in a copper polycrystal. Continuous stress application results in a coarsened microstructure quite different from that produced under residual stress conditions.

10:15 AM *W6.6

COMBINED ATOMISTIC AND MESOSCALE SIMULATION OF GRAIN GROWTH IN NANOCRYSTALLINE THIN FILMS.

Dorel Moldovan, Dieter Wolf, Simon R. Phillpot and Andrew J. Haslam, Materials Science Division, Argonne National Laboratory, Argonne, IL.

We have combined molecular-dynamics simulations with mesoscopic simulations to study the mechanism and kinetics of grain growth in a thin film of nanocrystalline palladium with a columnar grain structure. 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. The presence of both grain-boundary migration and grain rotation introduces a physical length scale, R_c , into the system. The growth process is characterized by two regimes: if the average grain size is smaller than R_c , grain growth is grain-rotation dominated; by contrast, growth is dominated by grain-boundary migration for grain sizes greater than R_c . Our study reveals that the growth exponents characterizing the power-law time dependence of the average grain size are different for the two growth regimes. We discuss how this methodology can be extended to allow the study of deformation process. This combination of atomic-level with mesoscopic simulations then enables the investigation of grain growth in systems containing a large number of grains and over long times in a physically realistic manner.

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

10:45 AM W6.7

MODELING THE EFFECTS OF TRIPLE LINE TENSION ON SURFACE GRAIN STRUCTURES. Jon Hilden, Raghavan Narayanan, and Alex King, Purdue University, Dept of Materials Science and Engineering, West Lafayette, IN.

A balance of surface energies exists where grain boundaries meet the surface of a flat solid specimen. The energy balance leads to grain boundary grooving on the surface, and the establishment of the equilibrium dihedral angle. While interior triple lines are defined at the intersections of three grain boundaries, exterior triple lines can be defined where grain boundaries meet the surface of the solid. Surface and interior quad points can likewise be defined at the intersections of four triple lines. Surface grooves are typically observed to be the deepest at the surface quad points. It has previously been hypothesized that triple lines exert line tension, causing surface quad points to recede further into the solid than would be expected from considerations of grain boundary energies alone. In this work, a simple model is constructed of hexagonal grains in a thin sheet using Surface Evolver numerical software. The equilibrium groove depths at surface quad points are investigated as a function of triple line tension. Results show that triple line tension does not appreciably affect grain boundary groove depths for any reasonable values of line tension. Results are discussed relative to preliminary experimental measurements using atomic force microscopy (AFM). The authors gratefully acknowledge the support of NSF grant number DMR0096147.

11:00 AM W6.8

COUPLED GROOVING AND MIGRATION OF INCLINED GRAIN BOUNDARIES. Huifang Zhang, Harris Wong, Louisiana State Univ, Dept of Mechanical Engineering, Baton Rouge, LA.

Grain-boundary migration controls the growth and shrinkage of crystalline grains and is important in materials synthesis and processing. A grain boundary ending at a free surface forms a groove at the tip, which affects its migration. This coupled grooving and migration is studied for a straight, inclined grain boundary intercepting a horizontal free surface. Surface diffusion is taken to be the mass transport mechanism for grooving. Previous work on a groove migrating at constant speed suggests that the grain boundary is pinned if the inclination angle is small. We find that the grain boundary is never pinned. The coupled motion can be separated into two time regimes. In regime I, both the grain-boundary and groove profiles grow with time following similarity laws. The groove profile is symmetric about the groove root. The symmetry forces the grain boundary to turn vertically at the tip, and this bending drives the migration. The self-similar profiles are shown to be linearly stable, and they grow continuously into regime II. In regime II, the turning relaxes following two different paths depending on σ/β , where β is the initial inclination angle of the grain boundary and σ is the supplementary dihedral angle ($\pi - \sigma$ is the dihedral angle). For $\beta > \sigma/6$, the groove root coordinates (x_0, y_0) $(t^{1/2}, t^{1/6})$ as time $t \rightarrow \infty$, whereas for $\beta < \sigma/6$, (x_0, y_0) $(t^{1/4}, t^{1/4})$. These results come from asymptotic expansions and agree with a finite-difference solution of the coupled equations. They show that the grain boundary is never pinned. The asymptotic solutions also apply to the Sun-Bauer method of measuring mobility, and predict grain-boundary profiles that agree better with experiments.

11:15 AM W6.9

TEMPERATURE EFFECTS ON ANISOTROPIC GRAIN GROWTH IN ALUMINUM. M. Upmanyu, Computer Science and Mathematics Department, Oak Ridge National Laboratory and Materials Science Program, Division of Engineering, Colorado School of Mines, CO; H. Zhang, D.J. Srolovitz, Department of Mechanical and Aerospace Engineering and Princeton Materials Institute, Princeton University, Princeton, NJ; B. Radhakrishnan, Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN.

Anisotropy in grain boundary mobility and energy can be very important in determining microstructural evolution. In this study, we examine the misorientation and temperature dependence of the $\langle 111 \rangle$ tilt grain boundary mobility and energy using atomistic simulations. Molecular dynamics simulations are carried out on U-shaped half-loop bicrystals. The activation energy and pre-exponential factor describing steady-state boundary mobility and the boundary energy vs. misorientation show cusps at misorientations corresponding to high symmetry grain boundaries. We also find that increasing the temperature changes the depth of the cusps. The effect of such temperature dependent changes on the nature of anisotropy in boundary properties on grain growth are investigated using three-dimensional Monte Carlo based Potts model simulations.

11:30 AM W6.10

LARGE SCALE STATISTICS FOR COMPUTATIONAL VERIFICATION OF GRAIN GROWTH SIMULATIONS WITH EXPERIMENTS. Melik C. Demirel^{1,2,3}, Andrew P. Kuprat², Denise C. George², Galen K. Straub², Amit Misra³, Kathleen Alexander³, Anthony D. Rollett¹. ¹Carnegie Mellon University, Department of Materials Science & Engineering, PA. ²Theoretical Division, Los Alamos National Laboratory, NM. ³Materials Science and Technology, Los Alamos National Laboratory, NM.

It is known that by controlling microstructural development, desirable properties of materials can be achieved. The main objective of our research is to understand and control interface dominated material properties, and finally, to verify experimental results with computer simulations. We have previously showed a strong similarity between small-scale grain growth experiments and anisotropic three-dimensional simulations [1] obtained from the Electron Backscattered Diffraction (EBSD) measurements [2]. Using the same technique, we obtained 5000-grain simulations from an Aluminum-foil with a columnar grain structure. Experimentally obtained starting microstructure and grain boundary properties are input for the three-dimensional grain growth simulation. In the computational model, minimization of the interface energy is the driving force for the grain boundary motion [3]. The computed evolved microstructure is compared with the final experimental microstructure, after annealing at 550°C.

References:

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11:45 AM W6.11
RECENT DEVELOPMENTS IN SIMULATING GRAIN GROWTH WITH MONTE CARLO ALGORITHMS. Qiang Yu, Sven K. Esche, Stevens Institute of Technology, Department of Mechanical Engineering, Hoboken, NJ.

The basic Monte Carlo (MC) method has previously been adapted to model grain growth and recrystallization. Its various modifications were employed to predict the grain growth kinetics, the grain size distribution and topology, and the influence of particle dispersion and anisotropic grain boundary energies for grain growth. In this work, the original two-dimensional MC algorithm for single phase normal grain growth was adapted to simulations with isotropic and anisotropic grain boundary energies. These developments were based on the fundamental idea that the grain growth process is a free energy reduction process, and thus in every step of the MC simulations a minimum-energy state of the lattice should be achieved. Accordingly, new procedures for selecting the lattice sites and orientations were developed and implemented. It had been shown theoretically that if the assumption of self-similarity is satisfied, then the grain growth should follow a parabolic law. The modified algorithm presented here generates time-invariant normalized grain size distributions for isotropic normal grain growth and correctly reproduces the kinetics of the microstructure evolution. In addition, it leads to significantly higher computational efficiency compared with previous implementations of the MC algorithm. Also, a recent re-examination of the original unaltered MC algorithm showed that in the early stages of the simulation the data fluctuate significantly around a parabolic curve. This effect may cause the results of the regression analysis on the domains including these local fluctuations to be seriously distorted, thus explaining the lower grain growth exponents often reported previously. Furthermore, grain growth with various models for the anisotropic grain boundary energy potential was simulated using the modified MC algorithm. Reasonable grain morphologies were obtained in all cases. Provided that the initial distribution of orientations is random, the parabolic growth law observed in the isotropic case remains unchanged, and the degree of anisotropy affects the grain growth rate only. These results further confirm earlier theoretical predictions.

12:00 PM W6.12
EVOLUTION OF MICROSCOPIC TO MESOSCOPIC SCALE OF DAMAGE IN HOT DEFORMATION. A.K. Ghosh, Dept of MS&E, The University of Michigan, Ann Arbor, MI.

Most engineering alloys, microstructurally similar to composite materials, have mixtures of hard and soft phases such as dispersions of particulates or laminae, their concentrations varying from dilute to highly concentrated mixtures. Deformation processing of such materials by rolling, forging and sheet forming to fabricate desired shapes invariably leads to incompatibility of plastic flow in the microscale, causing formation and growth of internal damage. Defect build-up starts at internal interfaces from initial sizes below the resolution of optical microscope, i.e., well into the submicroscopic range, to sizes that are several grain diameters wide, i.e. in the mesoscopic range. Such phenomena are linked with constraints to plastic flow at the interface, triaxiality of stress state and local strain concentrations. After fabrication, often such defects are large enough to directly influence the structural performance of the material. Success in the application of engineering materials in service is directly related to size and distribution of manufacturing defects, and thus an understanding of the damage evolution process is important. Prediction and control of defect size during manufacture of high performance structural components is a serious need for industry. This paper will present a status of damage evolution during high temperature processing of engineering alloys via modeling of constrained plasticity near void.

SESSION W7: MICROSTRUCTURAL EVOLUTION II
Chair: Slava Solomatov
Thursday Afternoon, April 4, 2002
Golden Gate C2/C3 (Marriott)

1:30 PM W7.1
THE EFFECT OF INTERPARTICLE FRICTION ON THE COMPACTION OF PARTICLES: AN FEM/DEM STUDY. Antonios Zavaliangos, Department of Materials Engineering, Drexel University, Philadelphia, PA.

Discrete element studies of powder compaction have been popular recently. A disadvantage of this technique is the need for simplification of the inter-particle contact behavior. To overcome this

problem, we analyze the compaction of powder by a 2-D finite element study of the compaction of 200 particles, each of which is discretized at a sufficient level to provide adequate detail of the interparticle interaction (a total of 60000 elements). The material is modeled as elastic-perfectly plastic. Simulations in an isostatic pressure and uniaxial strain (close die) mode show that the effect of interparticle friction on the pressure density relation is present only in the early stages of compaction. Differences are observed in the geometry of pores which in turn may affect material properties.

1:45 PM W7.2
AN INTERNAL VARIABLE PLASTICITY MODEL FOR SIMULATION OF SINTERING. Michael Braginsky, Veena Tikare, Sandia National Laboratories, Albuquerque, NM.

The concepts of sintering theory have been developed either based on the application of complex diffusion mechanisms to a simple geometry, or in the framework of continuum mechanics (i.e., plastic or nonlinear-viscous compaction of porous bodies). We present an internal variable plasticity model for simulation of sintering. Microstructural evolution characterized by 'spins' or phase orientations is simulated using modified statistical Monte-Carlo approach. This model is capable of simulating vacancy diffusion along grain boundaries, annihilation of vacancies at grain boundaries resulting in densification, and coarsening of microstructural features under the influence of the stress-strain state caused by vacancy annihilation. The model predicts both microstructural evolution and deformation of the sintering part. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under the Contract DE-AC04-94AL-85000.

2:00 PM W7.3
MODELING MICROSTRUCTURAL EVOLUTION DURING SINTERING IN A COMPLEX POWDER COMPACT. Veena Tikare, Michael V. Braginsky, Sandia National Laboratories, Albuquerque, NM; Eugene A. Olevsky, San Diego State University, San Diego, CA.

A kinetic, Monte Carlo model, capable of simulating microstructural evolution during sintering in 2D and 3D powder compacts, has been developed. Unlike most sintering models, this model can simulate microstructural evolution in systems consisting of hundreds of particles of arbitrary shapes and sizes. The model makes no assumptions of the geometry of the systems. Rather it simulates several microstructural evolution processes simultaneously in response to the local geometry. It can simulate curvature driven grain growth, pore migration and pore coarsening by surface diffusion, and densification by diffusion of vacancies to grain boundary and annihilation of these vacancies. Morphological changes and densification kinetics were used to verify the model. We will present the results of this model, discuss its capabilities and the utility of the results for other models. We will also discuss the limitations of this model.

2:15 PM W7.4
MESO-MACRO MODELING OF DIMENSION AND DAMAGE EVOLUTION IN SINTERING. Eugene Olevsky, San Diego State University, Dept of Mechanical Engineering, San Diego, CA; Veena Tikare, Sandia National Laboratories, Albuquerque, NM; Andrey Maximenko, Catholic University of Leuven, Leuven, BELGIUM.

Sintering distortions of composite powder structures are determined based upon the continuum theory of sintering implemented in a 3-D finite element computer code. The macroscopic constitutive parameters of the powder material are obtained on the basis of the meso-scale simulations of a realistic grain-pore structure. The model follows both the densification and the damage development during sintering using a new fracture criterion for the prediction of macroscopic strength in sintering. The simulation results are compared with the experimental data on sintering of multilayer ZnO and Cu powder composites.

2:30 PM W7.5
MODELING THE DIFFUSION-CONTROLLED GROWTH OF NEEDLE AND PLATE-SHAPED PRECIPITATES. Z. Guo, W. Sha, Metals Research Group, School of Civil Engineering, Queen's University of Belfast, Belfast, UNITED KINGDOM.

Various theories have been developed to describe the diffusion-controlled growth of precipitates with shapes approximating to needles or plates. The most comprehensive one is due to Ivantsov, Horvay and Cahn, and Trivedi (HIT theory), where all the factors that may influence the precipitate growth, i.e. diffusion, interface kinetics and capillarity, are accounted for within one equation. However, HIT theory was developed based on assumptions that transformation strain/stress and interfacial free energy are isotropic, which are not true in most of the real systems. An improved growth

theory of precipitates of needle and plate shapes was developed in the present study. A new concept, the compression ratio, was introduced to account for influences from the anisotropy of transformation strain/stress and interfacial free energy on the precipitate morphology. Experimental evidence supports such compression effect. Precipitate growth kinetics were quantified using this concept. The improved HIT theory (IHIT theory) was then applied to study the growth of Widmanstätten austenite in ferrite in Fe-C-Mn steels. The calculated results agree well with the experimental observations. In addition, attempts were made to estimate the value of compression ratio theoretically. Keywords: Precipitate kinetics, Precipitate growth, Compression ratio, Transformation strain/stress, Anisotropic interfacial free energy.

2:45 PM W7.6

GROWTH AND RIPENING OF CLUSTER DISTRIBUTIONS. Benjamin J. McCoy, Department of Chemical Engineering and Materials Science, University of California, Davis CA; Giridhar Madras, Department of Chemical Engineering, Indian Institute of Science, Bangalore, INDIA.

Ostwald ripening is the final stage of a first-order phase transition for condensation of a metastable phase. The first stage is nucleation, either homogeneous (a free energy barrier is surmounted to form critical-sized clusters) or heterogeneous (nucleation sites present in the system allow molecular, i.e., monomer, deposition). The second stage is cluster growth by monomer deposition, which depletes the metastable phase of monomer and causes stable clusters to grow regardless of their size. Owing to the random deposition of monomers from the metastable phase, this growth process yields a size distribution of clusters, even when the critical-sized clusters formed by homogeneous nucleation have the same uniform mass. Thus, a range of different sized clusters evolve over a range of time scales. Ripening occurs near equilibrium conditions when larger clusters grow at the expense of dissolving smaller clusters. We have proposed [G. Madras, B.J. McCoy, J. Chem. Phys. 115, 6699 (2001)] that ripening kinetics for growth and dissolution can be represented by a general population balance equation (PBE) for the cluster size distribution (CSD). This PBE can also describe cluster growth or dissolution in the absence of ripening. The Kelvin equation provides the effect of interfacial energy on solubility in terms of the cluster radius. The continuity equation conventionally applied to ripening or cluster growth is obtained as a Taylor series expansion of the governing PBE. Numerical and moment solutions of the PBE show the evolution of the CSD. The cluster number density declines, and the average cluster mass increases. The variance can initially increase as the CSD broadens by growth of large clusters, and then decrease until eventually vanishing. The final state after a long time is a single large cluster in equilibrium with the fluid solution. We will extend this model, which has been limited to size-independent rate coefficients for growth and dissolution, to include the effect of mass-dependent rates.

3:30 PM W7.7

MULTIPLICATIVE NOISE IN MICROSTRUCTURE EVOLUTION. K.G. Wang, M.E. Glicksman, and P. Crawford, MS&E Department, Rensselaer Polytechnic Institute, Troy, NY.

Understanding microstructural behavior is important because it controls mechanical, thermal, and electrical properties of engineering materials. A well studied example of microstructural evolution is phase coarsening. Lifshitz and Slyozov, and Wagner (LSW) formulated the kinetics of phase coarsening by excluding all interaction among particles, and ignoring local environmental information. LSW and other mean-field theories predict only global properties of phase coarsening, and cannot reveal local aspects. Computational simulation capable of predicting both local and global properties of aged microstructures were carried out. We modeled multiparticle diffusion equations to simulate the dynamics of the phase coarsening. Local environmental information and particle interactions are included in our simulations. These studies reveal that the growth rates of particles with the same radii can differ, and that particles with the average radius can grow, shrink, or remain conditionally stable. These results are in contrast to mean-field predictions. Multiparticle simulations prove that fluctuations occur in the particle growth rates, even at extremely low microstructural densities. We found that multiplicative noise provides a good basis to describe these fluctuations. Some recent progress in simulating microstructure evolution and multiplicative noise will be provided.

3:45 PM W7.8

NETWORK FORMATION BY SELF-ORGANIZED SUPRAMOLECULAR THREADS. Mehmet Sayar¹, S. I. Stupp^{1,2}.

¹Dept of Materials Science and Engineering; ² Dept of Chemistry, Medical School, Northwestern Univ, Evanston, IL.

Recent experiments in our group on self-organized networks provide a novel approach for creating bulk structures and surface patterns.

These networks have a two level hierarchical structure. Oligomers with multiple chemical blocks self-organize into supramolecular threads, which inter-connect to form the network. Monte Carlo simulations have been used to understand the formation and structural properties of these networks. The model gelators have two kinds of weak interactions (e.g., hydrogen bonding and π - π stacking), one governing self-organization into threads and the other providing inter-thread connectivity. The network structure has been studied as a function of concentration of gelators, the strength of interactions, and the stiffness of the molecular threads. The possibility of using these self-organized threads for creating surface patterns has been explored with 2-D simulations.

4:00 PM W7.9

COARSE STABILITY AND BIFURCATION ANALYSIS USING KINETIC MONTE CARLO SIMULATORS. Alexei Makeev, C. William Gear, and Ioannis G. Kevrekidis, Department of Chemical Engineering & PACM, Princeton University, Princeton, NJ; Dimitrios Maroudas, Department of Chemical Engineering, University of California, Santa Barbara, CA.

We implement a computer-assisted approach that, under appropriate conditions, allows the bifurcation analysis of the coarse dynamic behavior of microscopic simulators without explicitly deriving closed macroscopic equations for this behavior. The approach is inspired by the so-called time-stepper-based numerical bifurcation theory. We illustrate the approach through the computation of both stable and unstable coarsely invariant states for kinetic Monte Carlo models of three simple surface reaction schemes. We quantify the linearized stability of these coarsely invariant states, perform pseudo-arc-length continuation, detect coarse limit-point and coarse Hopf bifurcations, and construct two-parameter bifurcation diagrams. We also demonstrate a suite of 'coarse integration' schemes based on the so-called Projective Integrators we recently developed. The idea here is to use several parallel short bursts of microscopic simulations in order to extrapolate the longer-time behavior of the system moments. Finally, the extension of the above schemes to spatially distributed simulations will be discussed, with examples ranging from reaction-diffusion systems to chemotaxis.

SESSION W8: POSTER SESSION

Thursday Evening, April 4, 2002

8:00 PM

Salon 1-7 (Marriott)

W8.1

FUNDAMENTAL PROPERTIES OF THE SOLID EQUATION OF STATE INFERRED FROM SHOCK WAVE PHYSICS. Francis Chaiassé, Olivier Heuzé, CEA-DIF, Bruyères-le-Chatel, FRANCE.

The linear shock-velocity U versus particle velocity u , which is well suited for describing the Hugoniot curve of metals, is revisited from the thermodynamical point of view. By this way, we set-up a theoretical relation between the Grüneisen coefficient and the isentropic derivatives to third order at the initial state before jump, ensuring the linear $U(u)$ relation. When applied to the classical Morse potential describing the equation of state in a Mie-Grüneisen form, the theoretical result is in a good acceptance with the shock experimental results carried out on solids.

W8.2

NUMERICAL BIFURCATION ANALYSIS USING DETERMINISTIC ATOMIC-SCALE SIMULATION: STRESS-INDUCED INSTABILITIES AND STRUCTURAL TRANSITIONS IN CRYSTALS. Dimitrios Maroudas, Department of Chemical Engineering, University of California, Santa Barbara, CA; Ju Li, Sidney Yip, Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, MA; Frederick Milstein, Departments of Mechanical Engineering and Materials, University of California, Santa Barbara, CA; and Ioannis G. Kevrekidis, Department of Chemical Engineering & PACM, Princeton University, Princeton, NJ.

Systematic studies of nonlinear dynamical system response upon operating parameter variation rely on numerical bifurcation analysis. Traditionally, computational implementation of bifurcation theory has been based on models that employ partial differential equations for continuum-level descriptions of dynamical systems. In this presentation, we extend numerical bifurcation analysis to the study of dynamical systems with atomistic degrees of freedom (coordinates of individual atoms), such as complex materials with defects and nanostructural features. To demonstrate the methods of analysis, we focus on the structural response of a defect-free crystal to the application of external stress and the systematic mapping of the crystal mechanical stability boundaries. Specifically, an augmented

state+parameter space representation is implemented through pseudo-arc-length continuation for tracing asymptotic states of the classical equations of motion, according to classical interatomic potentials for atomic bonding in metals. The technique will be demonstrated through molecular-statics computations of true steady states in the zero-temperature limit; special emphasis will be placed on contraction mappings that do not require evaluation and inversion of a Jacobian matrix, such as quasi-Newton and conjugate-gradient iterative methods. Extension to analysis of higher-temperature behavior based on molecular-dynamics simulation will also be discussed. Results will be presented for the elastic stability and structural response of an EAM model of iron and a Morse model of nickel under uniaxial [100] tensile and compressive loading. The applied stress component is the bifurcation parameter and the corresponding response diagrams are strain-stress curves. In the former case, the response diagram exhibits two regular turning points that mark bcc-fcc structural transitions (Bain transformation), while in the latter it also exhibits branching of secondary deformation paths from the primary one. In all cases, the critical points are located accurately, the stability of the solution branches is determined, and the loss of crystal stability along the primary deformation path is demonstrated.

WS.3

MODELING AND NUMERICAL SIMULATIONS OF MICRODIFFRACTION FROM DEFORMED CRYSTALS.

Rosa Barabash, Gene Ice, Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, TN.

Brilliant synchrotron microprobes, offer new opportunities for the analysis of stress/strain and deformation distributions in crystalline materials. Polychromatic x-ray microdiffraction is emerging as a particularly important tool because it allows for local crystal-structure measurements in highly deformed or polycrystalline materials where sample rotations complicate alternative methods; a complete Laue pattern is generated in each volume element intercepted by the probe beam. Although a straightforward approach to the measurement of stress/strain fields through white-beam Laue microdiffraction has been demonstrated, a comparable method for determining the plastic-deformation tensor has not been established. Here we report on modeling efforts that can guide automated fitting of plastic-deformation-tensor distributions in three dimensions. It has been shown for example, that near a Bragg reflection $I(hkl)$, the reciprocal-space intensity distribution $I(q)$ exhibits characteristic behavior that depends on the local plastic-deformation-tensor. If an excess of edge dislocations of one sign $n+$ is formed, then long-ranged lattice rotations are induced that result in elongated (streaked) Laue reflections. The direction, asymmetry and magnitude of the streaking is sensitive primarily to unpaired edge dislocations, but can also be influenced by local rotation fluctuations introduced by the total number of dislocations (paired and unpaired). The presence of dislocation walls can be detected under certain conditions and local gradients in the dislocation density can be resolved both through differential aperture methods and through characteristics in the diffraction pattern. In general, the observed Laue pattern depends on the orientation of the diffraction vector, the active dislocation system(s), gradients in the dislocation density, and in elastic strain gradients. Modeling these effects is an essential first step towards automated fitting methods aimed at recovering three dimensions distributions of deformation structure.

Work sponsored by the Division of Materials Sciences. Oak Ridge National Laboratory (ORNL) is operated by UT-Battelle, LLC, for the U.S. Department of energy under contract DE-AC05-00OR22725. The submitted abstract has been authored by a contractor of the U.S. Government under contract DE-AC05-00OR22725. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

WS.4

COMPUTATION OF ION CONCENTRATIONS IN HYDRATING OPC/SILICA FUME MIXTURES USING CEMHYD3D. R.J. van Eijk, H.J.H. Brouwers, Dept of Civil Engineering, University of Twente, Enschede, THE NETHERLANDS.

In this paper CEMHYD3D model, originally developed the by NIST, is used for prediction of alkali, calcium, hydroxyl and sulphate pore water concentrations in hydrating ordinary Portland cement (OPC) and OPC/silica fume mixtures. Degrees of hydration, fractions of C-S-H and (water filled) porosity were computed using CEMHYD3D. Taylors model was used to describe release and sorption of alkalis into the pore water. The binding capacities of cementitious C-S-H and pozzolanic C-S-H with respect to sodium and potassium were determined according to binding experiments done by Song and Glasser. Incorporating this information into CEMHYD3D, alkali concentrations could be computed as a function of hydration time. Concentrations of the other ions were computed as a function of

hydration time, considering a small set of relevant solid equilibria: the portlandite + gypsum equilibria and the portlandite + ettringite + hydrogarnet equilibria. Reardon provided the used activity products and Pitzers method for calculating activity coefficients is employed. Results were compared with pore water measurements reported in literature, yielding good agreement.

WS.5

THREE-DIMENSIONAL MODELING OF ANISOTROPIC STRESS EFFECTS IN THERMAL OXIDATION OF SILICON. Xiaopeng Xu, Norbert Strecker, Victor Moroz, Avant! Corporation, Fremont, CA.

Thermal oxidation of silicon involves the following phenomena: 1) oxidant diffusion through the existing oxide layer, 2) oxidation reaction at the silicon/oxide interface, and 3) volume expansion of the newly grown oxide. The mechanical stress plays an important role in all three events: the diffusivity and reaction rate are strongly stress dependent, and the final oxide geometry is determined by the stress equilibrium. To accurately model thermal oxidation of silicon, stress analysis needs to be performed carefully. In our three dimensional process simulator finite strain kinematics is invoked to account for large deformation associated with oxide growth. Crystal elasticity is used to model anisotropic mechanical properties of silicon. The oxide is modeled as viscoelastic material and the stress history dependent relaxation is governed by the Maxwellian laws. At the silicon/oxide interface, the reaction activation barrier is taken as the product of hydrostatic pressure with activation volume that incorporates crystal anisotropy. The reactive boundary movement is tracked by solving a level set equation. To validate our model, thermal oxidation of non-planar silicon surfaces is simulated and compared with experimental observations. For a shallow trench isolation, the shape of the silicon/oxide interface at the upper corner is critical for the MOSFET source-to-drain leakage current and the shape at the lower corner affects the electric field distribution. TEM pictures have shown a distinctive $\{111\}$ facet at the corners along silicon/oxide interface but conventional models fail to predict the formation of these facets. Using our model described above, the facet formation is predicted and the numerical results are in good agreement with experimental observations. With these and other comparisons between numerical and experimental results, we conclude that a sufficient level of accuracy has been achieved using the described set of physical and mechanical models in our process simulation tool for the predictive oxidation modeling.

WS.6

THE THRESHOLD FOR GROWTH OF NANOSCALE VOIDS IN FCC METALS. J. Belak, R.E. Rudd and E.T. Seppala, University of California, Lawrence Livermore National Laboratory, Livermore, CA.

The threshold stress for void growth is an important parameter in nucleation and growth models of ductile fracture [1]. Here, we examine the growth threshold for spherical nanoscale voids ($1\text{nm} < \text{Diameter} < 10\text{nm}$) in copper using an EAM molecular dynamics model [2]. This threshold occurs when dislocations nucleate on the $\{111\}$ slip systems intersecting the void surface at about 45 degrees, where the shear stress is maximal. The framework of Rice-Thompson-Beltz [3] is used to analyze this dislocation nucleation in terms of the local stress and strain at the void surface and the lattice resistance to shear. The results are used to construct a model for growth of larger voids.

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- Acknowledgement: This work was performed under the auspices of the US Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

WS.7

PHASE SEPARATION IN ALUMINA-CHROMIA. Monique S.

McIntosh, Janet M. Hampikian, Thomas H. Sanders, Jr., School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA.

Since many high temperature alloys contain significant amounts of aluminum and chromium, it is important to fully understand the alumina-chromia phase diagram. Alumina and chromia are both protective oxides, in that diffusion through their oxide scales is slow and they generally have excellent adherence to their respective metals. Both alumina and chromia have the corundum crystal structure and share a common oxygen ion. The Al^{3+} and Cr^{3+} ions are also chemically similar with a size difference less than 15% according to the Shannon Prewitt scale for six-fold coordination[1]. As a result the alumina-chromia system shows complete mutual solubility and is represented by an isomorphous phase diagram. However, the alumina-chromia system exhibits an asymmetric miscibility gap under 1300°C . Using existing data from the literature, the alumina-chromia

system was assessed by thermodynamic modeling by Kim and Sanders[2]. They used regular and subregular solution models for the liquid and solid phases respectively, to define the phase boundaries for the miscibility gap in this system. Using this thermodynamic representation of the miscibility gap to select temperatures of interest, 75 m/o Al₂O₃ pellets were made and heat-treated for various times and temperatures. These experimentally observed microstructures are contrasted and compared to the compositions at the phase separation boundaries that are predicted by the model[2].

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W8.8

MOLECULAR DYNAMICS STUDY OF COMMENSURATE-INCOMMENSURATE PHASES IN HEXAMETHYLENE-TETRAMINE SUBERATE. Yuansheng Pan, Gervais Chapuis, Institute of Crystallography, University of Lausanne, SWITZERLAND; David Brown, University of Savoie, FRANCE.

Hexamethylene-tetramine suberate is an commensurate structure higher than room temperature and an incommensurate structure below that temperature, which has been solved from single crystal x-ray diffraction data. A molecular dynamics simulation of this system was carried out from 15 K to 580K. A second-generation consistent forcefield (CFF), was used to describe the interactions between atoms. In order to account for deficiencies in the forcefield, a compensating pressure tensor field was applied during the simulation. The experimental structure at 298K was taken as the starting structure and the phase transitions were investigated over all temperature range. A high symmetry commensurate structure was found between 410K and 290K and a low symmetry lock-in phase was observed below 150K. For temperatures lower than 290K, a new periodicity appears in the structure. An incommensurate structure appears between the high and low symmetry phases between 290K and 150K. The new periodicity associated with the incommensurate modulation is due to the appearance of additional long range ordering of the carbon chains. The present molecular dynamics simulation reproduces well the experimental x-ray diffraction results and gives new insight into the origin of the commensurate-incommensurate phases transition.

W8.9

GRAIN BOUNDARY GROOVING BY SURFACE DIFFUSION WITH STRONG SURFACE ENERGY ANISOTROPY. Tinghui Xin, Harris Wong, Louisiana State Univ, Dept of Mechanical Engineering, Baton Rouge, LA.

Facets appear often on crystalline solids, and need to be accurately modeled in studying surface evolution. A new model of facets has been developed recently in which a facet is represented by the Dirac delta function [1]. This model allows arbitrarily strong anisotropy in surface energy, but avoids the ill-posedness in evolution problems commonly associated with strong anisotropy. We incorporate this new model in studying grain-boundary grooving by surface diffusion. We consider partially to fully faceted surfaces with different facet orientations and 3, 4, and 6 fold symmetry in surface energy. We find that in all the cases the groove profile grows following a similarity law. We will present the faceted groove profiles and discuss their implications.

[1] T. Xin and H. Wong, "A δ -function model of facets," Surface Science 487, L529-L533 (2001).

W8.10

MODEL CALCULATION OF CONTACT AND BULK ELECTRIC TRANSPORT PROPERTIES OF GRANULAR HTSC. Vasily Omeltchenko, Galina Orlova, Alexey Sukhanov, Institute of Radioengineering and Electronics RAS, Frjazino, Moscow Reg., RUSSIA.

Electrical properties of normal metal contact to percolation Josephson HTSC medium are studied by computer simulation. The network of weak links with wide spread of critical currents is examined as a model of a granular superconductor. To describe weak links we used current-voltage characteristics (CVC) and temperature dependencies of critical current typical for Josephson junction. CVC and resistance-temperature (RT) dependencies are calculated. It is shown that near the critical current both bulk and contact CVC and RT dependencies follow $\ll 3/2 \gg$ law. The contact CVC and RT dependencies are broadened in comparison with the proper bulk characteristics. A peaks on the current and temperature dependencies of spreading resistance were found out. It is shown that these peaks were caused by nonuniform current distribution in nonlinear medium. Applicability of the effective medium model for description of the contact and bulk characteristics of HTSC media is demonstrated. The computer simulation results are in accord with experimental data obtained for contact Au-contact to Y-ceramics and for breakjunction contacts.

W8.11

MODEL COMPOUND VULCANIZATION AND IGC AS PREDICTION TOOLS IN CARBON BLACK EFFECT ON VULCANIZATION. Eduard Vidal-Escales, M. Paz Diago, Salvador Borros, Material Science Lab, Department of Physical Chemistry, IQS, Universitat Ramon LLull Barcelona, SPAIN.

The high specific surface area and concentration of carbon black (CB) in a rubber formulation has a great influence on the final mechanical properties. Furthermore, that influence can be observed as well during the vulcanization process. However, looking through literature there seems to be a lack of information related to the role of CBs in vulcanization reaction. Recently, our group has demonstrated the influence of CB in the accelerator decomposition using Model Compound Vulcanization (MCV) approach (1). The present work is focused on the application of MCV approach and Inverse Gas Chromatography (IGC) to predict the role of carbon blacks (CB) on vulcanization. Squalene was choosed as model molecule of natural rubber to undergo the vulcanization in presence of carbon black. This methodology gives rise to several advantages. On one hand, the model allows following the accelerator, vulcanization intermediate compounds, and even the crosslinked model molecule. Moreover, the similarity between the model and the polymer chain allows further extrapolation to discover the real samples performance. In order to complete the information required IGC analysis was used. IGC has been performed using both dispersive and specific probes to elucidate a wide range of CB surface active sites. The application of this new tool to a special type of carbon black (Durex-0) revealed two important effects: a shortening in the scorch time and a slightly increase of the cure rate. Such technique could also be applied to the particular case of a series of partially- polyaniline coated carbon blacks. In this case the following prediction could be drawn: The larger the amount of polyaniline coating of CB particles, the shorter the scorch time and the higher the vulcanization rate. This predicted behavior has been checked and verified with real formulations in both cases.

[1] S. Borrús, World Amazon Rubber Conference, Manaus (Brasil) 1999.

W8.12

NUMERICAL SIMULATION OF MICROSTRUCTURAL EVOLUTION OF LAMELLAR ALLOYS: APPLICATION TO Pb-Sn SOLDER. Rifa El-Khozondar, Viatcheslav Solomatov, New Mexico State Univ, Dept of Physics, Las Cruces, NM; Veena Tikare, Sandia National Laboratories, Numerical Modeling and Simulation, Albuquerque, NM.

Understanding the morphological changes of Pb-Sn solder alloys helps to improve their performance in electronic applications. The focus of our study is degeneration of lamellar structures at high temperatures. Microstructural evolution of the Pb-Sn eutectic lamellar structure is modeled numerically using Monte Carlo Potts approach. The initial structure consists of alternating layers of Pb-rich and Sn-rich phases, simulating the lamellar array in a near eutectic system. Faults are introduced to destabilize the system. After a short incubation period the shape of lamellae become irregular. The perturbations grow with time and eventually break the lamellae into nearly equiaxed grains. The grain size of the degenerated structure is 2-3 times the original lamellar spacing weakly depending on the spacing between the faults. This is consistent with the experimental observation of degeneration of Pb-62 wt% Sn solder. The duration of degeneration processes is comparable with the time it would take Ostwald ripening to produce grains of the same size. Eventually grain growth reaches the asymptotic regime of coarsening described by a power-law function of time.

W8.13

MODELING AND PHOTOABSORPTION STUDY OF YPd_{2-x}Rh_xB₂C SUPERCONDUCTORS. L.-S. Hsu, Dept of Physics, National Chang-Hua University of Education, Chang-Hua, TAIWAN; Y.K. Wang, G.Y. Guo, Dept of Physics, National Taiwan University, Taipei, TAIWAN; M.-D. Lan, Dept of Physics, National Chung Hsing University, Taichung, TAIWAN.

The electronic structures of six polycrystalline borocarbide superconductors YPd_{2-x}Rh_xB₂C (x=0, 0.05, 0.1, 0.15, 0.2, and 0.25) are studied by theoretical modeling and by photoabsorption spectroscopy around the Pd L_{III} edge. The calculation is a self-consistent all-electron full-potential linearized augmented-plane-wave method, and is based on the first-principles density-functional theory with the local-density approximation and generalized gradient corrections. The wavefunctions, the charge densities, and the potentials are expanded in terms of spherical harmonics inside the muffin-tin spheres. The Brillouin-zone integration is carried out by using the improved tetrahedron method. The effect of Rh substitution of the Pd atoms is taken into account by

the virtual-crystal approximation. The calculated Pd L_{III} x-ray absorption near-edge spectra and the Pd s plus d partial density of states (DOS) for these intermetallic compounds agree well with the corresponding experimental absorption spectra. The calculated total DOS curves for these compounds are compared with the valence-band spectra. The calculated total DOS values at the Fermi level are used to explain the higher superconducting transition temperatures found in these intermetallics.

W8.14

Abstract Withdrawn.

W8.15

DIRECT METHOD FOR MODELING SOLIDIFICATION AND MICROSTRUCTURE. Nicolay Bodyagin, Sergey Vikhrov, Stanislav Mursalov, Igor Tarasov, Ryazan Radioengineering Academy, Ryazan, RUSSIA.

Our previous investigations show that solidification can be describe as self-organization processes. Materials structure is spatially inhomogeneous, 'frozen', nonequilibrium system examined from the point of view of the nonlinear dynamics. Traditional approaches to the analysis of this system in terms of statistical characteristics such as spatial spectrum, correlation scale, and the like don't give information about its deterministic origin. Possibility of use of the known in nonlinear dynamics approach Takens for investigation of the structure order to be proved. The essence of method is that order in the system can be discovered by the sequence of measurements of any characteristic of the system. The measurements will be carried out with discrete intervals of time (length). On this data are defined: dimension of phase space, fractal dimension (FD) of attractor, Lyapunov exponents and other dynamical invariants. The objects of investigation were are silicon-based films, carbon, gallium arsenide, wolframite the surface profile obtained by of the scanning tunneling microscopy and atomic power microscopy. These data were processed according to Takens method by the Grassberger-Procaccia algorithm. The FD and its dependence on the embedding dimension were defined. Analyses of these data show that, surfaces structure have complex, determined chaotic character with many levels, and can be described by limited number of order parameters. By these results the algorithms for direct modeling of micro- and macrostructures and to control of growth processes were processed. The analytical connection between parameters of structure and dynamical characteristics of solidification, is established.

W8.16

SIZE AND GEOMETRICAL EFFECTS OF POLYCRYSTALS AND THIN FILM/SUBSTRATE IN MICRO-INDENTATION TEST. Yueguang Wei, Shan Tang, Manhong Zhao, LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing, CHINA.

Micro-indentation tests at scales on the order of sub-micron have shown that measured hardness increases strongly with decreasing indent depth or indent size, which is frequently referred to as the size effect. Simultaneously, at micron or sub-micron scale, another kind of effects, which is referred to as the geometrical effects such as crystal grain size effect, thin film thickness effect, etc., is also important to influence the measured material hardness. In the present research, the micro-indentation experiments for polycrystal Al and for Ti/Si₃N₄ metal thin film/ ceramic substrate system are carried out, when the crystal grain size and the thin film thickness are at the order of the size effect sensitive zone. Meanwhile, for comparing with the pure size effect, the micro-indentation experiments for single crystal W, Cu and Al are also carried out. The size effect and the geometrical effect are displayed experimentally. It is well known that the size and geometrical effects are at odds with the size-independence implied by conventional elastic-plastic theory. In the present researches, a kind of discrete dislocation method is used to model the composition effects from size effect and geometrical effect for polycrystal material and metal thin film/ceramic substrate systems when materials undergo micro-indenting. By comparing the theoretical predictions with experimental measurements, the values and the variation trends of the micro-scale parameters included in the discrete dislocation theory are predicted.

W8.17

THE SIMULATION OF COPPER DRIFT IN SiO₂ DURING BIAS TEMPERATURE STRESS (BTS) TEST. Jang-Yeon Kwon, Ki-Su Kim, Young-Chang Joo, Ki-Bum Kim, Seoul National Univ, School of Materials Science and Engineering, Seoul, KOREA.

By bias temperature stress (BTS) test the diffusion of copper in inter-metal dielectric material (IMD) has been investigated for a reliable copper interconnection. However because the solubility of copper is too low to be detected by Energy Dispersive Spectrometer (EDS) or Rutherford Backscattering Spectrometry (RBS), it is hard to study the behavior of copper during BTS test. Although Secondary

Ion Mass Spectrometry (SIMS) detects copper, a lot of analysis is required for precise observation of copper drift because statistical analysis is indispensable in BTS test and various low-k materials has been studying for high-speed device. Therefore, the simulation could be an effective approach for quantitative study of copper behavior during BTS test. The evolution of copper concentration in SiO₂ was simulated by solving diffusion equation which is derived by the flux of concentration and electric potential gradient because copper drift as an ionized state. By using simulated concentration of copper, flatband voltage shift as a function of BTS time was simulated. Although the simulated flatband voltage shift was overestimated compared with reported experimentally result, this deviation could be eliminated by simulation of copper concentration considering the variation of electric potential due to copper ions in SiO₂. In order to evaluate the effect of driving forces on copper diffusion during BTS test, the numbers of copper diffused by concentration and electric potential gradient were compared. It is considered that the driving force of concentration gradient is negligible over 1.0MV/cm, however, the number of copper forced by concentration gradient is nearly same with that by electric force at the condition of device working (0.1MV/cm). Because the concentration profile of copper when electric failure occurs varies strongly with not temperature but electric field, it is thought that Fowler-Nordheim tunneling controls leakage current during BTS test.

W8.18

RELAXOR BEHAVIOR OF RANDOM DIPOLE SYSTEM IN THE HOST LATTICE WITH STRONG POLARIZABILITY. A. Artemev, Department of Mechanical and Aerospace Engineering, Carleton University, Ottawa, Ontario, CANADA; S.V. Semenovskaya, and A.G. Khachatryan, Department of Ceramic and Materials Engineering, Rutgers University, Piscataway, NJ.

A model describing the system of local dipoles which are randomly distributed in the host lattice with high dielectric susceptibility is developed. The local dipoles are produced by off-center dopant ions that have six equivalent off-center locations producing different orientations of dipole moment. The time-averaged dipole moment of each local dipole is determined by the occupation numbers for these locations. The interaction between local dipoles is produced through the polarization of the host lattice generated by local dipoles. An effective Hamiltonian is obtained for the dipole-dipole interaction and employed for the derivation of the Master Equation describing the evolution of the filling numbers, the time-averaged dipole moment of local dipoles, and the average polarization of the system. Computer simulation has been performed for systems with different concentrations of off-center dopant ions in a wide range of temperatures and with static and alternating applied fields. The computer simulation shows that at low concentrations of off-center dopant ions the paraelectric state transforms at a low temperature to the macroscopically paraelectric state consisting of randomly oriented polar clusters. These clusters amplify the effective dipole moment and drastically increase the dielectric constant. A broad peak of dielectric susceptibility is obtained at the transition temperatures. At intermediate dopant concentrations, the material undergoes a diffuse phase transition to the ferroelectric state smeared within the temperature range. A further increase in the dopant concentration makes the transition sharper and closer to the conventional ferroelectric transition. The polarization vs. applied field hysteresis loops are obtained in relaxor and ferroelectric states subjected to alternating applied field. The obtained results are compared with the behavior of the KLT relaxor ferroelectric K_{1-x}-Li_x-Ta-O₃.

W8.19

EFFECT OF PARTICLE POLYMER INTERFACE AND MICROSTRUCTURAL CHARACTERISTICS ON THE MECHANICAL BEHAVIOR OF A COMPOSITE. Rajesh Raghavan, Craig Carter, Massachusetts Institute of Technology, Department of Materials Science and Engineering, Cambridge, MA.

The mechanical behavior of a polymer composite depends on the combined characteristic relaxation times of its constituents as well as its microstructural length scales. Rigid-particle-filled polymer composites with various microstructures and material components have been analysed with an image-based finite element approach. We obtain direct results for the macroscopic deformation properties for composites with specified components and therefore can analyze the correlation between the polymer composite microstructure and the macroscopic mechanical behaviour. Virtual dynamical mechanical analysis and strain rate tests provide insight into the role of microstructure on the average mechanical properties and their variations. The characteristics of the polymer filler interface properties is shown to have a large effect on macroscopic deformation behaviour. We present results on the interplay of multiple structural relaxation time scales that are inherent in the polymer composite material and its effect on the macroscopic properties.

W8.20

HOW DO MARTENSITIC TWIN BOUNDARIES MOVE?

Graeme Ackland and Udomsilp Pinsook, Dept. of Physics and Astronomy, University of Edinburgh, Edinburgh, UNITED KINGDOM.

The essence of multiscale modelling is to integrate out the unnecessary detail from small scale simulation to build a model at a larger lengthscale. Nowhere is this more problematic than at the atomic level, where treatments at the atomic scale pass to those treating only the relevant defects. The central problem becomes identification of the relevant defects. Results of molecular dynamics calculations (MD) are presented to address the mechanism by which martensitic twin boundaries move in NiTi and Zr. An interatomic potential is used which reproduces relevant experimental and ab initio data. Samples of twinned, defective martensitic microstructure are prepared by MD cooling from the austenite phase. These samples are then subjected to external strain, which causes deformation by twin boundary motion. Several features emerge identifying the objects which should be considered in a higher level model. Twin boundaries comprise segments of low index boundaries and geometrically necessary dislocations. Low energy, atomically smooth boundaries are immobile (and also incompatible with the transformation strain). The geometrically necessary dislocations are sessile, their Burgers vector being at an angle to the twin plane. Unstable, mobile twin boundary dislocations are emitted and absorbed from the geometrically necessary dislocations, the motion of these defects enables twins to move. Finally, the effect of ordering in removing ambiguities in the austenite - martensite mapping and suppressing conventional dislocation motion is demonstrated.

SESSION W9: DEFECT FORMATION & MIGRATION, SURFACES, GROWTH AT SURFACES

Friday Morning, April 5, 2002
Golden Gate C2/C3 (Marriott)

8:00 AM *W9.1

RELAXATION OF COMPRESSED ELASTIC ISLANDS ON A LIQUID LAYER. Z. Suo, J. Liang, R. Huang, Mechanical and Aerospace Engineering Department and Princeton Materials Institute, Princeton, NJ; H. Yin, J.C. Sturm, Electrical Engineering Department and Center of Photonics and Optoelectronic Materials, Princeton University, Princeton, NJ; K.D. Hobart, Naval Research Laboratory, Washington, DC.

A technique has been developed recently to fabricate SiGe film islands on a glass layer, which in turn lies on a silicon substrate. The islands are initially under an inplane compressive strain. Upon annealing, the glass flows and the islands relax. The resulting strain-free islands can be used as substrate to grow epitaxial optoelectronic devices. This paper models the annealing process. A small island relaxes by inplane expansion. Because of the viscosity of the glass, the relaxation starts at the island edges, and moves toward the island center. A large island wrinkles before the inplane relaxation reaches the center. After some time, the wrinkles may disappear when the inplane relaxation arrives. Alternatively, the wrinkles may cause tensile stress in the island, leading to fracture. We model the film island by the von Karman plate theory, and the glass layer by the Reynolds lubrication theory. The solid and the fluid couple at the interface by traction and displacement continuity. The inplane displacement and the vertical deflection evolve simultaneously. A combination of experiments and calculations describes the conditions under which the islands relax by inplane expansion without significant wrinkling. For further details, see <http://www.princeton.edu/suo/>

8:30 AM W9.2

ATOMISTIC SIMULATION OF SURFACES, GROWTH AND MORPHOLOGY OF INORGANIC MATERIALS. S.C. Parker, D.J. Cooke, S. Kerisit, N.H. de Leeuw, S.E. Redfern, Department of Chemistry, University of Bath, Bath, UNITED KINGDOM.

Computer simulation represents a reliable tool for studying the properties of inorganic materials at the atomic level. The advantage of an atomic level description is that the influence of different additives, impurities and defects on the structure, stability and reactivity can be examined. Thus atomistic simulations provide a useful complement to experiment by aiding in the characterization of materials and for predicting the behavior of new materials. In this talk we aim to illustrate the scope and limitations of these simulation methods by describing some of our recent work on modeling the surfaces of ceramics and minerals at the atomic level using a combination of ab initio and molecular modelling techniques. For example, one of the difficulties when comparing with experiment is that water is often present at the surface of 'real' materials. Thus we have begun to investigate the effect of water on the surface structure and stability

for a range of materials. Success with modeling the water-oxide interface means that we can begin to model growth and dissolution and perhaps more significantly suggest ways in which these processes can be modified. By focusing on two materials, CaCO₃, calcite and Fe₃O₄, magnetite we will show how the simulations can model, first, the structure of the crystal surfaces, secondly the energetics of crystal growth and finally, the morphology of these materials. The good level of agreement for both the predicted surface structures and the predicted macroscopic morphologies gives us confidence in the reliability of the techniques.

8:45 AM W9.3

TRANSITION LAYER AND DEFECT FORMATION AT SOLID/LIQUID INTERFACE OF SILICON: A MOLECULAR DYNAMICS STUDY. T. Motooka and K. Nisihira, Kyushu University, Dept of Materials Science and Engineering, Fukuoka, JAPAN.

Almost all Si wafers for microelectronics device applications are produced by the Czochralski (CZ) method in which crystal growth is initiated by supercooled liquid through crystal pulling of melted Si in a silica crucible. It has been known that voids and extended interstitials with a size of ~ 1000 Å are formed in CZ grown Si wafers. These defects are called grown-in defects and considered to become problematic in future Si microelectronics devices. It is also empirically shown that the defect type is determined by the ratio of V (pulling speed) to G (temperature gradient at the solid/liquid (s/l) interface), V/G ; i.e., there exists a critical value of $(V/G)_c \approx 0.1 \text{ mm}^2/\text{min K}$ and the vacancy (interstitial)-type defects are formed for V/G larger (smaller) than $(V/G)_c$. Although extensive studies have been carried out to analyze the V/G problem based on macroscopic diffusion equations of point defects, the detailed atomistic processes are not well understood. We have investigated atomic diffusion properties at the s/l interface of Si based on large-scale molecular-dynamics (MD) simulations using the Tersoff potential. It has been found that there exists a transition layer with a thickness of ~ 10 Å at the s/l interface where the atomic diffusion constant decreases from that of bulk-liquid Si. The result is consistent with high-resolution electron microscopy measurements. We also suggest that the V/G -dependence of the defect type described above can be attributed to non-equilibrium atomic diffusion in the transition layers. Examples of atomic motions at the solid/liquid interfaces during defect formation obtained by MD simulations will be shown by a movie.

9:00 AM W9.4

MODELING THE MECHANISM BEHIND SUPERCONFORMAL ELECTRODEPOSITION: VERSUS EXPERIMENT. Daniel Josell, Thomas Moffat and Daniel Wheeler, NIST, Gaithersburg, MD.

We describe the atomic-level mechanism by which changes of surface area during electrodeposition lead to local variations in coverage of adsorbed additives, inducing location-dependent metal electrodeposition rates and continuum micrometer-level superconformal filling of features. Simulations from a continuum model of this mechanism are compared to filling experiments for trenches ranging from 350 to 90 nm wide and 450 nm deep. We first identify electrolytes that yield superconformal electrodeposition of metal in trenches [1]. All kinetic parameters describing the rate of atomic-scale additive accumulation on metal surfaces and the impact of the accumulation on macroscopic metal deposition rates are obtained from studies of deposition on flat metal specimens. Kinetic parameters are found to be linear in the fractional coverage of the additive that accelerates the rate of metal-deposition, which saturates at one monolayer [2,3]. Accumulation of the dilute accelerator is described by diffusion across a boundary layer and deposition voltage dependent interface kinetics. Where specimens are not flat (i.e., non-zero curvature), area change during deposition causes additional change of local accelerator coverage through mass conservation. Accelerator coverage, and thus the deposition rate, at the bottoms of superfilling features is found to be dominated by this area change effect. The model uses a geometrical simplification that captures the area-reduction/coverage-increase mechanism while simplifying the problem to solution of coupled differential equations. With no free parameters, the model predicts filling behavior of lithographically patterned features. Predictions are in excellent agreement with experimental results; initial period of conformal growth, subsequent superfill, and development of overfill bump are all observed and explained as fill versus void formation for different deposition voltages, electrolyte compositions and feature dimensions [2-4].

1. T.P. Moffat, J.E. Bonevich, W.H. Huber, A. Stanishkevsky, D.R. Kelly, G.R. Stafford and D. Josell, *J. Electrochem. Soc.*, 147, 4524 (2000).
2. T.P. Moffat, D. Wheeler, W.H. Huber, and D. Josell, *Electrochem. Solid-State Lett.*, 4, C26 (2001).
3. D. Josell, T.P. Moffat, D. Wheeler and W.H. Huber, *Phys. Rev. Lett.* 71, 016102 (2001).
4. D. Josell, D. Wheeler, W.H. Huber, J.E. Bonevich and T.P. Moffat,

A Simple Equation for Predicting Superconformal Electrodeposition in Submicrometer Trenches, J. Electrochem. Soc. (in press).

9:15 AM W9.5

NUMERICAL SIMULATION OF SUPERCONFORMAL ELECTRODEPOSITION USING THE LEVEL SET METHOD.

Daniel Wheeler, Daniel Josell, Thomas P. Moffat, NIST, Gaithersburg, MD.

A model for superconformal electrodeposition is implemented using the level set method. Superconformal filling of trenches and vias occurs when a high aspect ratio feature on a silicon wafer fills without voids or seams. The general principal behind this phenomena is known as the Curvature Enhanced Accelerator Coverage (CEAC) mechanism and has been described extensively. The model presented here utilizes the level set method (LSM) to track the position of the copper/electrolyte interface as the features are filling. The LSM maintains a scalar variable as a distance function whose zero level set marks the position of the interface allowing accurate determination of the curvature. The LSM has been used previously for similar applications in integrated circuit fabrication such as etching, deposition and lithography. The novelty in the work presented here, involves the accurate determination of the accelerator surface coverage at the interface. The coverage depends on both adsorption from the electrolyte and interface arc length evolution. The additive surface coverage in turn determines the velocity of the front. In the numerical method a scalar variable is used to hold the value of the surface coverage at nodal points close to the interface. The fast marching method, a subset of the LSM, is employed for maintenance of the distance function and building of extension velocities. The LSM algorithm is embedded in a Finite Volume framework that allows solution of the electrolytes species determined by diffusion through the electrolyte. Additional species and other physical phenomena, such as fluid flow, can be added with relative ease. Several test cases are examined to validate the LSM and surface coverage model. Trench and via superfilling simulations will be presented and compared with both simple analytical models and experiments.

9:30 AM W9.6

A CONTINUUM MODEL FOR ANISOTROPIC EPITAXIAL LATERAL OVERGROWTH. Mikhail V. Khenner, Richard J. Braun, Dept. of Math Sciences, University of Delaware, Newark, DE; Michael G. Mauk, AstroPower, Inc., Newark, DE.

We developed a consistent mathematical model for the crystal growth on a substrate covered by the mask material with a periodic series of parallel long trenches where the substrate is exposed to the vapor phase. Surface diffusion and the flux of particles from vapor are assumed to be the main mechanisms of growth. The model consists of two PDEs; one for the crystal surface dynamics and one for the surface concentration of atoms on the mask. A geometrical approach to the motion of crystal surface in two dimensions is adopted and nonlinear evolution equations are solved by a finite-difference method. The model allows the direct computation of the crystal surface shape, as well as the study of the effects due to mask regions of effectively nonzero thickness. As in experiments, lateral overgrowth of crystal onto the mask and enhanced growth in the region near the contact of the crystal and the mask is found, as well as the comparable crystal shapes. The growth rates in vertical and lateral directions are investigated. Results for both isotropic and anisotropic growth will be reported.

9:45 AM W9.7

MODELING SURFACTANT EFFECTS ON HETEROGENEOUS THIN FILM GROWTH. Hongmei Wen, Matthew Neurock, University of Virginia, Dept of Chemical Engineering, Charlottesville, VA.

The addition of metal or organic surfactants can significantly alter the properties and growth of thin films. These surfactants alter the kinetics and in some instances the actual mechanisms for surface diffusion. This can lead to marked changes in the structural, magnetic and electronic properties of deposited films. In the processing of Cobalt-Copper multilayers, surfactants have been used to reduce interfacial roughness and mixing. But the mechanisms of surfactants effects are still not very clear. In this work, we have used ab initio density function theory of spin polarized GGA potential to elucidate the mechanisms. Noble metals, like Ag and Au, with nearly filled d-bands, show significantly lower barriers for diffusion and promote diffusion of Cu and Co. For example, the diffusion barrier for Cobalt to step down a homogeneous Cobalt edge is 0.204 eV. However, after introducing 25% surfactant into the step edge, the step-down activation energy of Cobalt become 0.151 eV for Co-Ag system, and 0.115 eV for Co-Au system. Therefore, this reduces interfacial roughness and promotes the thin film properties.

10:30 AM W9.8

SIMULATION OF DEFECT FORMATION DURING THE

IRRADIATION OF VANADIUM ALLOYS. L.A. Zepeda-Ruiz, S. Han, R. Car, D.J. Srolovitz, G.J. Ackland, Princeton Materials Institute, Princeton University, Princeton, NJ; B.D. Wirth, Chemistry and Materials Directorate, Lawrence Livermore National Laboratory, Livermore, CA.

Radiation damage in metallic alloys leads to the simultaneous development of a distribution of point defect clusters and solute redistribution. In the present study, we examine these effects in a potential vanadium-based first wall fusion reactor alloy. The key elements to such a calculation are accurate descriptions of the key point defects, molecular dynamics simulations of the displacement cascade, and kinetic Monte Carlo simulations of the evolution of the point defect distributions. The fundamental point defect (vacancy, tetrahedral and octahedral interstitials, $\langle 111 \rangle$ crowdion, and $\langle 111 \rangle$, $\langle 110 \rangle$, and $\langle 100 \rangle$ split interstitials) properties (formation energies and migration barriers) are first determined using first principles methods. Simulations based on existing empirical interatomic potential predict point defect stability that is in stark contrast to those from the first principles calculations. Therefore, a new interatomic potential for vanadium is developed. We employ this new potential in molecular dynamics calculations of the displacement cascades associated with 14 MeV neutron irradiation. Atomistic and first principles simulations are also used to determine all of the parameters needed for the kinetic Monte Carlo simulations of the evolution of the point defect distributions.

10:45 AM W9.9

MULTISCALE MODELING OF POINT DEFECTS NEAR INTERFACES AND FREE SURFACES IN THIN FILMS. Vinod Tewary, NIST, Materials Reliability Div, Boulder, CO.

Many physical properties of thin films depend upon the presence of point defects such as vacancies and interstitials and their elastic interactions with the interface between the film and the substrate and the free surfaces. Whereas the macroscopic continuum model can be applied to calculate the strain field due to extended defects such as the interfaces and free surfaces, a model for point defects must account for the discrete atomistic structure of the crystal lattice. A Greens function method is described for multiscale modeling of point defects at the atomistic level and free surfaces and interfaces at the macroscopic level in the same formalism. We use the lattice static Greens function for atomistic modeling of a point defect. The advantage of the lattice static Greens function is that it is semi-analytic and can model a large crystallite containing about a million atoms with no excessive CPU requirement. The lattice static Greens function reduces asymptotically to macroscopic continuum Greens functions which we use to model free surfaces and interfaces. We use the virtual force method along with the asymptotic limit of the lattice static Green function to satisfy the continuity conditions at the interface and the zero traction boundary condition at the free surface. The resulting Greens function has the discrete atomistic behavior near the point defects and the macroscopic continuum behavior near the interface and the free surface. The method is applied to calculate the lattice distortion and strains in thin films of metallic and semiconductor crystals containing vacancies and also the elastic interaction between a vacancy, the interface and the free surface.

11:00 AM W9.10

LARGE-SCALE MOLECULAR DYNAMICS SIMULATIONS OF INTERSTITIAL DEFECT DIFFUSION IN SILICON.

David A. Richie, Department of Physics, Ohio State University, Columbus OH; Jeongnim Kim, NCSA/MCC, University of Illinois at Urbana-Champaign, Urbana, IL; Richard Hennig, Kaden Hazzard, Steve Barr and John W. Wilkins, Department of Physics, Ohio State University, Columbus, OH.

The simulation of defect dynamics and evolution is a technologically relevant challenge for computational materials science. The diffusion of small defects in silicon unfolds as a sequence of structural transitions. The relative infrequency of transition events requires simulation over extremely long time scales.

We simulate the diffusion of small interstitial clusters (I_1, I_2, I_3) for a range of temperatures using large-scale molecular dynamics (MD) simulations with a realistic tight-binding potential. A total of 0.25 μ sec of simulation time is accumulated for the study. A novel real-time multiresolution analysis (RTMRA) scheme extracts meta-stable structures from the dynamics that are easily identified and cataloged. The validity of these meta-stable structures are verified with more accurate first-principles calculations. The same RTMRA techniques automatically detect and characterize transition events. This information is used along with nudged elastic band calculations for the exploration of relevant reaction paths.

This comprehensive approach to the study of small interstitial clusters lays the groundwork for a global view of defect evolution and diffusion. *Supported by NSF, DOE and SRC with computational resources of OSC, NCSA and NERSC.

11:15 AM W9.11**MULTISCALE MODELING OF STRESS-DEPENDENT DIFFUSION IN SILICON: AB-INITIO CALCULATIONS.**

Wolfgang Windl, Ohio State Univ, Dept of Materials Science and Engineering, Columbus, OH; Murray S. Daw, Clemson Univ, Dept of Physics, Clemson, SC; Neil N. Carlson, Physical Sciences Research Laboratory, Motorola, Inc, Los Alamos, NM; Matthew Laudon, Axiowave Networks, Marlborough, MA.

Traditionally, it has been assumed that the major effect of substrate stresses were dislocation formation and response, whereas stress effects on diffusion were thought to be negligible. With the reduction of gate lengths and the use of more exotic gate materials, stress-mediated diffusion becomes a more prevalent component in determining the final dopant profile and subsequent device performance. We have developed a complete methodology to simulate the effects of general anisotropic non-uniform stress on dopant diffusion in silicon. The macroscopic diffusion equation is derived from microscopic transition state theory, the microscopic parameters are calculated from first principles, and feature-scale stresses are modeled based on stress measurements as a function of temperature. A continuum solver combines the ingredients into an engineering-level model. In this paper, we present ab-initio calculations for diffusion mechanisms and stress-dependent diffusion tensors for boron and arsenic diffusion in silicon. Our prediction of the stress dependence of implanted dopant profiles under a gate stack is in good agreement with experiments.

11:30 AM W9.12**THEORY OF DIFFUSION UNDER STRESS IN INTERSTITIAL ALLOYS AND SIMULATION OF SEGREGATION FORMATION NEAR DEFECTS.** Maria Ganchenkova, Andrei Nazarov, Moscow Eng Phys Inst, Dept of Materials Science, Moscow, RUSSIA; Alexander Mikheev, IP Bardin Central Res Inst of Ferrous Metallurgy, Dept of Metal Physics, Moscow, RUSSIA.

To describe the stress influence on diffusion flows in interstitial alloys, we use an approach, developed earlier for the case of vacancy mechanism. This approach, in opposite to most of other known ones, takes into account the atomic structure in the neighborhood of the defect and stress, that could modify the energy of jumping atom through the displacement field not only at site but and in saddle position. Apart from it, it takes the shear stresses into consideration that can modify the frequency of jumps through the displacement field at site and saddle position. Stress fields alter the surrounding atom configuration and, as a consequence, the height of the activation barrier is changed. Knowing these changes it is possible to calculate the jump rate and to obtain the expressions for the interstitial diffusion fluxes in fcc and bcc structures. In these nonlinear equations, influence of deformation tensor component on diffusion flux is determined by coefficients depending on atom interaction. For studying of interstitial redistribution near the defects, such as dislocation or crack orifice, we used two levels of simulation. First one is evaluation of mentioned coefficients. For this purpose we have developed a model into the framework of molecular static method taking into account an atom environment as near the interstitial as for the saddle-point configuration. The second level is modeling of interstitial segregation formation based on nonlinear diffusion equation taking both stress fields generated by defect and self-stresses into consideration. The simulation was done for the cases of H and C atoms in bcc metals near the crack orifice.

11:45 AM W9.13**KINETICS OF DEFECT COMPLEX FORMATION IN ORDERED STRUCTURES.** Maria Ganchenkova, Andrei Nazarov, Moscow Eng Phys Inst, Dept of Materials Science, Moscow, RUSSIA.

Intermetallic compounds are highly ordered alloys that constitute an important class of structural materials. To understand the behavior of mechanical properties under extreme operating conditions calls for fundamental studies of material properties. Of special interest are defect formation and migration processes, and interactions among defects that might lead to formation of defect complexes. In basis of present work it is laid the idea to take into account the influence of defect interaction on their diffusivities in full measure. Singularity of developed approach is logically checked combination of two types of methods. When the distance between two defects is small, the values of activation barriers of atom jumps calculate with help of molecular static method. But for the case of the larger distances we use developed approach, which allows to take into account the influence of elastic field on jump rate. Into the framework of this approach, it was obtained the expression for calculation of activation barrier change of atom jump in arbitrary direction. According to this expression the activation barrier value depends on the deformation tensor components, initial local atomic configuration near the jumping atom and saddle-point configuration. The components of deformation tensor are determined by anisotropic elastic field generated by another defect. Based on obtained values of activation barriers we calculate

the probabilities of atom jumps in arbitrary directions for different defect configurations. It allows us to realize the kinetics Monte-Carlo method for defect complex migration. As results of the simulation we can determine an average binding energy of defects and their diffusion coefficients. This approach was applied to the ordered structure of B2-type for the case of two interactive vacancies. The results show the formation of dynamic pair of these vacancies and their migration as tight complex, what confirm realization in such structures of Dynamic Pair mechanism.

SESSION W10: MODELING AT THE NANOSCALE

Friday Afternoon, April 5, 2002

Golden Gate C2/C3 (Marriott)

1:30 PM *W10.1**MULTISCALE FE/MD/QMD METHOD AND MULTIMILLION ATOM SIMULATIONS OF NANOSYSTEMS AND INTERFACES ON PARALLEL COMPUTERS.** Priya Vashishta, Rajiv K. Kalia, Aiichiro Nakano, Louisiana State Univ., Concurrent Computing Laboratory for Materials Simulations, Baton Rouge, LA; Elefterios Lidorikis, MIT, Physics Dept., Cambridge, MA; Martina E. Bachlechner, West Virginia Univ., Physics Dept., Morgantown, WV; Fuyuki Shimojo, Hiroshima Univ., JAPAN; Shuji Ogata, Yamaguchi Univ., JAPAN.

Unprecedented opportunities for remarkable advances in the next decade exist at the interface of information and nanotechnologies. On petaflop computers and on a Grid of geographically distributed parallel machines, we will be able to seamlessly (from atomic to macroscopic length scales) simulate, visualize, and interrogate technologically important nanostructured materials and nanoscale devices comprising biochemical systems/self-organized monolayers/metal-ceramic-semiconductor interfaces. Our multiscale atomistic simulation approach consisting of seamless integration of finite element (FE) method/molecular dynamics (MD) method/quantum molecular dynamics (QMD) method implemented with scalable and portable, space-time multiresolution algorithms will be presented. Multiscale approach for multimillion atom simulations has been used to investigate nanosystems and atomic-level stresses in semiconductor/ceramic interfaces.

2:00 PM W10.2**DISLOCATION ACTIVITY IN NANOCRYSTALLINE NI: A MOLECULAR DYNAMICS COMPUTER SIMULATION STUDY.** H. Van Swygenhoven, P.M. Derlet, Paul Scherrer Institute, Villigen, SWITZERLAND; M.J. Caturla, Lawrence Livermore National Laboratory, Livermore, CA.

It has been recognized for some time that the Hall-Petch relationship, which usually is explained on the basis of dislocation pileups at grain boundaries, must break down at grain sizes such that a grain cannot support a pileup. Large scale molecular dynamics simulations demonstrate that with increasing grain size in the nanometer regime, there is a shift from a purely inter granular deformation mechanism to one which also involves intra-granular mechanisms, via the nucleation and propagation of partial dislocations (Van Swygenhoven *et al* Phys. Rev. B **60** 22 (1999) and Phys. Rev. B (in press) (2001)). The present work investigates by means of molecular dynamics the onset and nature of the partial dislocations for a variety of grain sizes up to 30 nm under uniaxial tensile conditions and the increased dislocation activity when grain size increases. The possible existence and stability of a full dislocation is investigated as function of grain size. It is also shown that a thin film geometry does facilitate dislocation emission, which indicates that results from in-situ deformations in TEM has to be taken with caution (Derlet and Van Swygenhoven, Phil. Mag. A (in press) (2001)).

2:15 PM W10.3**CHARGE PATCHING METHOD TO GENERATE THE CHARGE DENSITY OF A NANOSTRUCTURE.** Lin-Wang Wang, NERSC, Lawrence Berkeley National Lab., Berkeley, CA.

Using the folded spectrum method, it is now possible to calculate the electronic states of a thousand to a million atom nanostructure, given that the single particle Schroedinger's equation of this nanostructure is known. Previously, we have been using empirical pseudopotentials to generate the potential in the Schroedinger's equation. However, for more reliability and accuracy, first-principle/selfconsistent quality potentials are highly desirable for many systems, ranging from impurity to large lattice mismatched alloys. We have developed a charge patching method to generate the charge density (hence the potential) of a large system from small prototype system first principle calculations, but without doing a direct first principle calculation for the large system. This method has been tested for N impurity in GaAs, general Fullerenes systems, and GaAsN alloys. The resulting charge densities are about 1% different from the direct first

principle calculated charge densities. The single electron eigen values differ by about 50 meV from the direct results, and the total energies differ by about 1-5 meV/atom.

3:00 PM W10.4

CALCULATION OF THE PHONON DISPERSION IN A SEMICONDUCTOR QUANTUM DOT CRYSTAL.

Olga L. Lazarenkova and Alexander A. Balandin, Univ of California at Riverside, Dept of Electrical Engineering, Riverside, CA.

Regimented three-dimensional (3D) quantum dot arrays, e.g. quantum dot crystals (QDC), attracted significant attention due to their modified density of electronic states and relaxed optical selection rules [1]. Several novel device applications have been recently proposed for such structures. Electron-phonon, photon-phonon, or phonon-phonon interactions normally define most of the material properties. In order to predict properties of QDC one needs to know the phonon dispersion of the structure. Although different types of QDC had already been fabricated, their vibration spectrum has not been studied yet. Thus, many predictions concerning electron-phonon transport in quantum dot arrays have been made on the basis of the qualitative assumption that the phonon should scatter more in such structures. In order to find the acoustic phonon dispersion in QDC we solved the elasticity equation for the continuum model with periodic boundary conditions using the finite difference method. Multiple scattering from three-dimensional regimented QD interfaces leads to folding of the linear bulk phonon dispersion with gaps on the edges of the quasi-Brillouin zone and deceleration of acoustic vibrations. Moreover, it creates "nearly" standing phonon modes in the dot or barrier regions. These modes have nonzero energy at the zero wave vector and may be considered as quasi-optical branches with characteristic energies much less than in the bulk. It may strongly affect the physical processes that involve photon-phonon interaction. We found that phonon-phonon scattering increases significantly in QDC because phonons may be in superposition state much more often than in bulk material. All transfer processes in the material depend on electron-phonon scattering. The calculated phonon dispersion allows us to compute the electron-phonon relaxation rates. Changing size of QD's, interdot distance and their regimentation one can tune phonon as well as electron dispersion. The latter creates an exciting opportunity to make a QDC structure with required combination of electronic and vibration properties.

[1]. O.L. Lazarenkova and A. Balandin, *J. Appl. Phys.*, **89**, 5509 (2001).

3:15 PM W10.5

DYNAMIC IMPURITY SEGREGATION IN FRACTURE.

Gerbrand Ceder, Anton Van der Ven, Dept of MS&E, MIT, Cambridge, MA.

It is generally accepted that impurities can have a significant effect on decohesion and fracture. In the past, first principles computations have been used to compute the force required to separate crystal planes (traction curves) with and without impurity segregation. In these studies the impurity concentration is generally not equilibrated with its sources (bulk or gas phase). In this work we develop a model to compute chemically equilibrated traction curves, whereby the local impurity concentration for any force and crystal-plane separation is equilibrated with a reservoir at constant chemical potential. We find that chemical equilibration qualitatively modifies the traction curves. Under constant chemical potential, the separation of crystal planes may occur at constant force. The maximum force required to separate planes is significantly reduced from when constant impurity concentrations are used. Interestingly, we find that the maximum stress for decohesion varies discontinuously with the impurity chemical potential, indicating that the fracture stresses may behave very non-linearly with impurity loading. These results indicate the importance of chemical equilibration in atomistic level simulations.

3:30 PM W10.6

A UNIFIED MODELING TECHNIQUE FOR MULTISCALE SIMULATION OF NANOSTRUCTURED MATERIALS.

Chunyu Li, Tsu-Wei Chou, University of Delaware, Newark, DE.

The science and technology have been developed into a nano-technology era. In this era, almost all physical properties of materials are size-dependent. Accompanied with the increasing of applications of nanoscale materials, multiscale simulation of materials become more important to study and design of devices involving nanostructured materials. But computations involving nanoscale structures are still a great challenge to the computational community. There is a urgent demand that we develop an efficient modeling technique for nanostructured materials just like the finite element method that great successfully used for designing and analyzing most engineering systems. In this paper, we extend the concept of computational structural mechanics into the atomistic modeling of covalently bonded nanostructures and propose a modeling technique

of molecular structural mechanics. In this model, a linkage between macroscopic structural mechanics and nanoscopic molecular mechanics is established. The fundamentals of our modeling are that covalently bonded nanostructures are essentially stable frame-like structures constituting of atoms. The primary bonds between two nearest-neighboring atoms act like load-bearing beam members, whereas an individual atom acts as the joint of the related load-bearing beam members. The sectional property parameters of these beam members can be obtained by establishing a linkage between structural mechanics and molecular mechanics. This modeling technique provides a unified approach for multiscale simulation of materials. It makes the transition from the macroscopic scale to the nanoscopic scale much smoother. Our computations show the computational efficiency of multiscale simulation using this modeling technique is several orders higher than existing methods.

3:45 PM W10.7

MODELING OF DISLOCATION INTERACTION WITH

PRESSURIZED VOIDS. Peihua Jing, Tariq Khraishi, Dept of Mechanical Engineering, Univ of New Mexico, Albuquerque, NM; Brian Wirth, Materials Science and Technology Division, Lawrence Livermore National Laboratory, Livermore, CA; Hussein Zbib, School of Mechanical and Materials Engineering, Pullman, WA.

Three-dimensional dislocation dynamics is used to study the interaction of dislocations with pressurized voids. Such a situation occurs in irradiated materials where Helium-filled "bubbles" interact with moving dislocations. The simulations involve a large number of voids and are thus computationally intensive. In the simulations, the stress field of each of the bubbles is provided from elementary elasticity theory. Such stresses enter directly into the calculation of the Peach-Koehler force acting on a dislocation segment and causing its motion. The simulation results show an undesired hardening behavior, as reflected in a stress-strain curve, associated with the existence of these voids. The flow stress of the material correlates with the number density of the voids. Dislocation dynamics appear to be a good numerical tool for studying the above irradiation problem.