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<td>Maria Bartelt, LLNL</td>
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<td>James Evans, Iowa State Univ</td>
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Symposium T Objective: To showcase recent developments in statistical mechanical modeling of non-equilibrium structures and processes in materials (including film growth, solidification processes, and bulk defect dynamics).

Symposium T Highlights: Statistical Mechanical Modeling in Materials Research, first highlighted current modeling strategies for epitaxial film growth and other complex processes at surfaces. Growth on low-index surfaces was described using: atomistic lattice-gas models predicting behavior in a specific system (Fig.1); level-set methods incorporating discrete layers but a continuum description of lateral morphology (C. Ratsch, UCLA); and (fully) continuum approaches describing evolution via stochastic PDE’s (M. Siegert, Simon Fraser U.). Step-wandering and bunching instabilities for growth on vicinal surfaces (A. Pimpinelli and A. Videcoq, LASMEA), and modeling of growth in complex semiconductor systems were also discussed. Other talks addressed optimum catalyst design (A.P.J. Jansen, Eindhoven U.) and propagation of reaction-fronts (akin to phase waves) in surface reactions (Da-Jiang Liu, Iowa State U.).

In the area of solidification, symposium T highlighted: the development of a new phase-field model of electrochemistry with potentially important application for electroplating (J. Guyer, NIST); molecular dynamic simulations that characterize for the first time the anisotropic capillary and kinetic properties of the solid-liquid interface in pure metals and simple binary alloys (M. Asta, Northwestern U. and J. Hoyt, Sandia-New Mexico); phase-field simulations of dendritic evolution in undercooled melts (Fig.2) and during directional solidification, that make use of the atomistically computed interface properties and of new powerful algorithms that extend the phase-field
approach into parameter ranges relevant for experiment (C. Beckermann, U. of Iowa); and the incorporation of fluid flow in three-dimensional phase-field simulations of dendritic growth (J. Dantzig, U. of Illinois).

The discussion of structures and properties induced by deformation centered on the development of new methods suitable for modeling realistic size systems and plastic strains (V. Bulatov, LLNL). Of particular interest is the emergence of characteristic length scales, as strain localizes in patterns of linear defects, be they networks of 'ridges' in crumpled candy paper (E. Kramer, Simon's Rock College), or 'loopons' (A. Finel, ONERA) and dislocation boundaries (W. Pantleon, Risoe NL) in deformed metals. Bridging between atomistic and continuum approaches, I. Groma (Etvs), J. StIken (LLNL), and A. El-Azab (PNNL) introduced stochastic theories for the evolution of materials stresses and dislocation densities during deformation. Other talks showed how fluctuations in these stresses and symmetries control the spatial characteristics of propagating fronts (M. Caturla, LLNL, Fig.3; D. Vandembroucq, CNRS) and branching cracks (L. Sander, U. Michigan).

Figure 3 — Snapshot of a molecular dynamics simulation of an initially spherical shock front developing square symmetry in a spherical fcc Cu crystal. After bouncing at the center of the ball the front produces a void (M. Caturla, LLNL).

Future Direction for Symposium T: Over the next several years, we expect to see substantial advances in capabilities for detailed and realistic statistical mechanical modeling of materials. This potential is driven by availability of ab-initio electronic structure codes (which provide input to the modeling), advances in accelerated-MD and large-scale Kinetic Monte Carlo simulation (coupled with increased computational power), theoretical advances in methods which connect-length-scales, etc. This Symposium will provide a natural venue to showcase and assess these general methods and developments, as well as their applications to a broad range of materials problems.


Organizers for Symposium T in 2001: Maria Bartelt (LLNL); James Evans (Ames Laboratory and Iowa State University); Alain Karma (Northeastern University); Salvatore (Princeton University), Dietrich Wolf (Universitaet Duisburg).

Report Prepared by: Maria Bartelt, James W. Evans, and Alain S. Karma

Date: 13 August, 2002
SYMPOSIUM T
Statistical Mechanical Modeling in Materials Research
November 25 – 29, 2001

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Proceedings to be published in both book form and online
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as Volume 701
of the Materials Research Society
Symposium Proceedings Series

* Invited paper
FT T: FUNDAMENTAL METHODS OF MULTISCALE MODELING  
Sunday, November 25, 2001  
9:00 a.m. - 5:00 p.m.  
Room 210 (Hynes)

The purpose of this tutorial is to introduce the many facets of multi-length-scale modeling. Because of the growing interest in the field of multiple length scale modeling, this tutorial will provide the attendees with a balanced description of the main facets of this field as applied in materials science. The tutorial will consist of four 45-minute lectures that will cover half a day, and the remaining time will be dedicated to a hands-on computer session where the attendees will have access to computers to run actual applications. The areas to be covered are the four fundamental areas that are required for multiple length-scale modeling: electronic structure theory, atomistic modeling (molecular dynamics and Monte Carlo methods), dislocation dynamics, and continuum level modeling. These lectures are meant to provide the attendees with a broad overview of the field and its challenges, and a detailed description of a particular method that will be utilized in the second part of the tutorial. The second half of the tutorial will be a hands-on session where personal computers will be used for the attendees to run illustrative examples in the four topical areas. There will only be a few computers, so attendees are encouraged to bring their laptops for use in the second part of the tutorial.

Instructors:  
Ronald Miller, Carleton University  
Geroge Gilmer, Lawrence Livermore National Laboratory  
Andrew Quong, Lawrence Livermore National Laboratory  
Russein Zibih, Washington State University

SESSION T1: MORPHOLOGICAL EVOLUTION DURING EPIТАКSY  
Chair: Vladimir Privman and Da-Jiang Liu  
Monday Morning, November 26, 2001  
Room 310 (Hynes)

8:30 AM *T1.1  
COARSENING OF MOUNDS IN EPITAXIAL GROWTH:  
CRystalline SYMMETRIES AND CHARACTERISTIC LENGTH SCALES. Martin Siegert, Academic Computing Services, Simon Fraser University, Burnaby, British Columbia, CANADA.

Formation of mounds and the coarsening of such morphologies in molecular beam epitaxy has been found to depend sensitively on the crystalline symmetries of the substrate: the coarsening law differs for deposition on (111) and (001) substrates. Furthermore, the length scale that can be used to characterize the growth law also depends on the substrate symmetry. For triangular symmetries there exists only a single length scale, the pyramid size, and the coarsening law \( R(t) \propto t^{1/2} \) can be found analytically. The solution even provides a good approximation for the prefactor \( c \). For quadratic symmetries there exist two competing length scales related to the densities of pyramid edges and so-called "roof-tops". The ratio of these densities has a crucial effect on the growth law. Finally, in the case of an isotropic substrate there exist several length scales the importance of which is still unclear.

9:00 AM *T1.2  
THE LEVEL-SET METHOD FOR MODELING EPIТАКSYAL GROWTH. C. Ratsch, N.E. Caffias, M. Petemen, M. Kang, UCLA, Los Angeles, CA; M.F. Gyure, HRL Laboratories, Malibu, CA; D.D. Vvedensky, Imperial College, London, UNITED KINGDOM.

We develop an island dynamics model that employs the level-set technique to describe epitaxial growth. This method is essentially continuous in the plane, yet it retains atomic discreteness in the height. In this method, the surface morphology is described by defining the island boundaries as the set \( \varphi = 0 \) of the so-called level-set function. Islands are nucleated on the surface and their boundaries are moved at rates that are determined by the adatom density, which is obtained from solving the diffusion equation. Reversible aggregation of adatoms can be included without any additional computational cost. Scaled island size distributions in the submonolayer aggregation regime are compared to those obtained from a kinetic Monte Carlo (KMC) simulation for irreversible as well as reversible aggregation. Excellent agreement is obtained. We identify spatial fluctuations in the seeding of islands as the only essential source of noise, while all other stochastic elements can be averaged.

We also show that the level-set method can naturally be extended to multilayer growth; here, the set \( \varphi = n - 1 \) corresponds to the \( n \)th layer. Roughening and coarsening of the surface will be discussed. In particular, we will study the evolution of the step edge density, which is related to the RHEED signal in experimental studies. A qualitative and quantitative comparison to KMC simulations will be given.

9:30 AM T1.3  
ATOMISTIC MODELING OF MOUND EVOLUTION DURING Ag/Ag(100) HOMOEPITAXY: THREE GROWTH REGIMES. K.J. Casperson, A.R. Layson, C.R. Stoldt, V. Fourteen, P.A. Thiel, J.W. Evans, Iowa State Univ, Ames, IA.

A realistic atomistic model is developed to describe VSST simulations of observation of mound formation in 25ML Ag/Ag(100) films deposited between 175K and 300K. The model is then used to interpret VSST data for kinetic roughening and mound coarsening, and to extend this analysis up to a few 1000ML. Three distinct growth regimes are found: initial transformation from 2D islands to 3D mounds; an extended mound steepening regime (of slow coarsening and rapid roughening); and finally asymptotic slope selection (with complex mound ordering, annihilation, and coalescence dynamics reflecting up-down symmetry breaking). These regimes are compressed at lower temperatures.

References:  

9:45 AM T1.4  
LEVEL SETS AND REVERSIBLE ISLAND GROWTH. Max Petersen1, Christian Ratsch2, Russel Caffias3, and Andrew Zangwill1. 1Georgia Tech, School of Physics, GA. 2UCLA, Dept. of Mathematics, CA.

The level set approach applied to the modeling of epitaxial growth allows a description which is discrete (atomistic) in the height profile and continuous in the lateral dimensions. Therefore, virtues of continuum and discrete models can be combined. The feasibility of this approach in the case of homoepitaxial growth with irreversible aggregation has been successfully shown [1]. In this model, island boundaries evolve with a velocity that is obtained by solving the diffusion equation. Here we present an extension to the island dynamics model to include reversibility, i.e., the possibility of thermal detachment of atoms from island edges. As a consequence, islands do not always grow, and break-up of islands is explicitly allowed in our approach. We make no assumptions about a critical nucleus. The island densities and island size distributions obtained within our model are in very good agreement to those calculated by kinetic Monte Carlo (KMC) simulations. The advantage of our model over the KMC consist in suppressing the simulation of irrelevant attachment-reattachment events by replacing them by their corresponding time average. Thus, an implementation of our model requires essentially no additional computational cost in comparison to the irreversible case. This feature is especially advantageous for the simulation of annealing and ripening. We will discuss the time evolution of the island densities and island size distributions during these processes.

References:  

10:30 AM T1.5  
SURFACE MORPHOLOGICAL STABILITY AND PATTERN FORMATION IN MODELS OF EPITAXIAL DEPOSITION. Alberto Pimpinelli, Arnoo Videoos, LASME, Université Clermont-Ferrand 2, FRANCE; Masha Vladimirova, IRRMA-EPFL, Lausanne, SWITZERLAND.

Controlling pattern formation at the surface of epitaxially growing crystals is an important technical and fundamental topic. In particular, morphological instabilities have to be understood to be avoided, or, possibly, exploited. A novel mechanism leading to the onset of surface instabilities during epitaxial growth on vicinal substrates is presented. It is based on the coupling between the surface densities of several diffusing species, in the presence of Ehrlich-Schwoebel barriers at step edges. These diffusion species may be precursor molecules (e.g. trimethylgallium) and adatoms (e.g. Ga adatoms) in chemical vapour epitaxy, or adatoms (e.g. Ga and As) and molecules (e.g. GaAs) in MBE. We investigate in large details a simple two-particle model accounting for this coupling, and we are able to show that, depending just on growth conditions, step flow growth in the same system may be unstable against either meandering or step bunching, as observed for instance in GaAs deposition on vicinals of GaAs(110). This is contrary to what happens in one-particle models for, say, molecular beam epitaxy, where Ehrlich-Schwoebel barriers always oppose step pairing during step flow growth, and are only able to induce meandering instabilities. This is, to our knowledge, the only model that predicts step bunching during homoepitaxial growth without invoking an unlikely "anti-Schwoebel" effect.
Heteroepitaxially grown semiconductor thin films are known to undergo 2D island formation. Recent observations also indicate that pit formation during growth may occur concurrently with the appearance of islands. We have recently observed the nucleation of 2D islands and pits during the growth of a series of In$_x$Ga$_{1-x}$As/GaAs (001) films using Molecular Beam Epitaxy. While it is generally understood that stress relief in strained films favors both island and pit formation, and that the proximity of islands to pits may be favored by stress-mediated interactions, the kinetics of the island-pit growth process that determine whether pits arise have not been investigated in depth. In order to understand the importance of adatom mediated interactions on pit formation during growth we have devised a theoretical model of island and pit nucleation during the growth of In$_x$Ga$_{1-x}$As alloy compounds. The model treats the formation of islands of the group III species as the rate-limiting step for island growth. Using kinetic equations we explicitly model the interactions of adatoms with surface steps and 2D islands in addition to their incorporation into 3D islands. The group V (As) chemical potential determines the relative free energies of islands and pits leading to different rates of nucleation of these features. The predictions of this model for the spontaneous formation of pits will be discussed.

We examine a class of step flow models of epitaxial growth obtained from a Burton-Cabrera-Frank (BCF) type approach in a (1 1)-dimensional setting. Our goal is to formulate an equivalent continuum model by passing to the continuum limit. Away from peaks and valleys, the continuum law is a Hamilton-Jacobi equation (HJE) for the evolution of the surface height. The peaks and valleys are free boundaries for this HJE; their evolution must be specified by suitable boundary conditions, reflecting the microscopic physics of the discrete model. At peaks, the governing physics involves nucleation. We study the peak boundary condition by performing numerical simulations of the step flow dynamics, using a simple but reasonable nucleation law. Our simulations reveal the presence of "traveling-wave-like" patterns in the profiles near the peaks. The relationship between these patterns and the continuum equation will be discussed. In particular, we shall address the importance of evaporation for matching the local behavior near the peak to the solution of the continuum equation.

Quantitative information on the kinetcs of step bunching from the distribution of terrace widths is analyzed. Anomalous vacancies and adatom migration are included. The model will be explored. The goal of the approach is to treat the complex geometry, including void formation, that occurs during plating in vias and trenches for on-chip metallization.

We present the first application of phase field modeling to electrochemistry. The phase field technique has previously been applied to the time evolution of complex dendritic, eutectic, and peritectic solidification morphologies. The present work was motivated by the mathematical analogy between the governing equations of solidification dynamics and electroplating dynamics. For example, the solid-liquid interface is analogous to the electrode-electrolyte interface. The various overpotentials of electrochemistry have analogues with the supercoolings of alloy solidification: diffusional (constitutional), curvature, and interface attachment. Dendrites can form during solidification and during electroplating. However, it is thought that solidification is more important than electroplating. Further, the inherent non-linear kinetics in electrodeposition is different from solidification, where problems are generally well-modeled with linear kinetics. The present model properly predicts the charge separation associated with the equilibrium double layer at the electrode-electrolyte interface and its extent in the electrolyte as a function of electrolyte concentration. The kinetic behavior of the model will be explored. The goal of the approach is to treat the complex geometry, including void formation, that occurs during plating in vias and trenches for on-chip metallization.

The phase field model incorporates both melt convection and thermal noise. A modified SIMPLE method is used to solve the conservation equations for flow. A multiple time step algorithm is developed, which uses a large time step for the flow field calculations while reserving a fine time step for the phase-field evolution. The operating state (velocity and shape) of a dendrite tip in a uniform axial flow is found to be in quantitative agreement with the prediction of the Obre-Vladimirov theory. The phase-field results for the complex interface problem of dendritic growth in a diffusive environment. The phase-field results for the complex interface problem of dendritic growth in a diffusive environment. The phase-field results for the complex interface problem of dendritic growth in a diffusive environment.
The phase-field method, based on continuum equations of Ginsburg-Landau type, has become the method of choice for numerical simulations of solidification patterns. Recent progress, both in mathematical analysis and numerical algorithms, makes it now possible to perform accurate three-dimensional simulations on computer relevant length and time scales. This will be illustrated by (i) the dendritic solidification of a pure substance, where the shape and velocity of the dendrite tips can be directly compared to experimental results for both low- and high-speed growth regimes, and (ii) the directional solidification of binary alloys, where the dynamics of cellular and eutectic patterns can be analyzed. Furthermore, in addition to solidification the phase-field method can also be applied to other free-boundary problems. We have developed a phase-field formulation for the classical BCF model of surface growth that is able to simulate the evolution of viscous surfaces on mesoscopic length and time scales, and that can be used to model epitaxial growth in the step-flow regime. We present results on the growth dynamics of spiral ridges that form around screw dislocations, and discuss possibility of generalizing the model to include Schoeckel barriers and elastic interactions.

Experimental and Numerical Study of Two-Phase Microstructure Formation during Directional Solidification of Dilute Binary Alloys: Bias Echebarria and Alain Karma, Northeastern University, Physics Dept, Boston, MA.

We study directional solidification of dilute binary alloys by means of a phase-field formulation. This avoids the problem of tracking the interface through the introduction of an order parameter, or phase-field φ, which varies smoothly from one value in the liquid to another in the solid across an interface region. However, the resulting equations are stiff, due to the disparity of scales between the interface thickness and the diffusion length. We use a recently derived phase-field model, whose thin interface limit yields a much less stiff restriction on the choice of interface thickness than previous formulations and permits to eliminate non-equilibrium effects at the interface. This allows us to make quantitative comparisons with experiments and study the onset of sidebranching and the cell to dendrite transition for realistic values of the physical parameters. Recently, it has been observed experimentally that increasing the externally imposed thermal gradient reduces the onset velocity and wavelength of sidebranching. We present simulations that confirm this counter-intuitive effect and study the onset of sidebranching as a function of the thermal gradient, pulling velocity and cell spacing.

Experimental and Numerical Study of Two-Phase Microstructure Formation in Peritectic Solidification. T. S. Lo, S. Dobler, M. Piap, A. Karma, and W. Kurs, Courant Institute of Mathematical Sciences, New York University, New York, NY; Department of Materials, Swiss Federal Institute of Technology, EPFL, Lausanne, SWITZERLAND.

We report the results of a combined experimental and numerical study of two-phase microstructure formation during directional solidification of peritectic alloys. The experiments are conducted in the Fe-Cu system that is ideally suited to investigate microstructural pattern formation in a predominantly diffusion-controlled growth regime due to the small density contrast between solid and liquid that minimizes the amount of convection in the melt. These experiments focus on a regime of large G/V (thermal gradient/growth rate) ratio where the solid-liquid interface of both solid phases is morphologically stable. The microstructures observed are eutectic-like (lamellar and rod) coupled growth structures and new "island banding" microstructures. The latter consist of rows of islands on one solid phase (Cu or primary) inside the continuous matrix of the other phase. The latter structures are observed either as transients that seed the formation of coupled growth structures, or as the final microstructure. On the modeling side, we use a sharp-interface boundary integral model to determine quantitatively the stability limits of coupled growth as a function of lamellar spacing, composition, and G/V ratio, and a diffuse interface phase-field model to investigate qualitatively the complex mechanisms involving both nucleation and growth that control the selection of island banding and coupled growth structures. We find an excellent overall agreement between experimental and numerical results.

Experimental and Numerical Study of Two-Phase Microstructure Formation in Peritectic Solidification. Bias Echebarria and Alain Karma, Northeastern University, Physics Dept, Boston, MA.
explains many properties of the latter which could not be previously understood. Thus, the colloid and nano-scale particle dispersions are interesting link between nanosize and micrometer size particles. It model of formation of uniform particles, by LaMer, and offers an recent theoretical explanation of this process expands the classical monodispersed colloids of various shapes, obtained by precipitation in synthesis involving nanosize particles and their new unique properties shapes, ranging in sizes from nanometer to colloidal, has been widely practiced. The importance of well-defined dispersions of particles of different catalysts for some simple model systems in which one reactant prefers to adsorb on one component of the catalyst and the other reactant on the other component. We show that there are many structures that can become the most reactive depending on the reaction conditions. The most reactive structure can be predicted without any calculations or simulations in some limiting cases using the concept of the rate limiting step, but in general this is not possible. We then use Dynamic (also called Kinetic) Monte Carlo simulation to describe the kinetics properly, and Genetic Algorithms to optimize the structure of the catalyst.

6:30 PM T3.2
FROM ATOMISTIC LATTICE-GAS MODELS FOR SURFACE REACTIONS TO HYDRODYNAMIC REACTION-DIFFUSION EQUATIONS. De-Jiang Liu, Ames Laboratory, Iowa State University, Ames, IA.

Local adsorption, desorption, reaction processes occurring in surface reactions, along with adspecies interactions and diffusion, produce a diverse variety of spatiotemporal pattern formation. Traditionally, this phenomenon has been tackled by mean-field (MF) reaction diffusion equation (RDE). A more fundamental approach is through the use of atomistic lattice-gas models, which can account for effects of adlayer ordering and fluctuations that are neglected in the MF-RDE approach. The pattern formation problem poses a challenge to direct simulations of lattice-gas models. At least for one of the adspecies, the diffusion process happens at a much faster time scale and larger length scale than all the other processes. Our strategy is to develop an appropriate (non-MF) RDE formulation to treat this "hydrodynamic" regime. This requires special simulation procedures, coupled with a correct description of chemical diffusion in mixed reactant adlayers. We apply this approach to a model CO oxidation system that exhibits bistability. The problem of chemical waves and equistability is studied.

9:00 PM T3.3
GROWTH OF MONODISPERSED COLLOIDS BY NUCLEATION AND AGGREGATION OF NANOSIZE SUBUNITS. Vladimir Privman, Department of Physics and Center for Advanced Materials Processing, Clarkson University, Potsdam, NY.

The importance of well-defined dispersions of particles of different shapes, ranging in sizes from nanometer to colloidal, has been widely recognized in applications and in basic studies of advanced materials. Our program endeavors to advance understanding of formation of uniform particles of simple and composite structure, with focus on synthesis involving nanosize particles and their new unique properties for dimensions smaller than the typical sub-monolayer colloidal scales. Presently, there is convincing experimental evidence that many monodispersed colloids of various shapes, obtained by precipitation in solutions, are formed by aggregation of such nanosize units. Our recent work on explanation of this process expands the classical model of formation of uniform particles, by LaMer, and offers an interesting link between nanosize and micrometer size particles. It explains some of the latter which could not be previously understood. Thus, the colloid and nano-scale particle dispersions are actually closely related, and we will emphasize uniform aspects of the dynamics of their formation in this presentation.

9:30 PM T3.4
A COMPUTATIONAL INVESTIGATION OF SELECTIVE MOVPE OF A1GaAs, AS IN THE PRESENCE OF HCI. Maria Nemirovskaya, Carlo Cavallotti, Klavs Jensen, MIT, Dept. of Chemical Engineering, Cambridge, MA.

The selective deposition of A1GaAs, as can be performed using MOVPE reactors with the deposition on the mask suppressed by the presence of HCI. The quality of the film and the shape of the features depend strongly on the gas phase composition, temperature and pressure. Multiscalar simulations were done in order to improve our understanding of the fundamental processes determining film growth and its morphology. Quantum chemistry calculations were performed to identify the key reactions between HCI and the A1GaAs, as surface as well as the gas phase precursors. A gas phase and surface kinetic scheme that is able to predict the growth of A1As and GaAs in the presence of HCI was thus developed and its validity was tested through the reactor scale simulations of the experimental data. Then the morphological evolution and the onset of the facet formation were studied using kinetic Monte Carlo model. Experimental literature rates of diffusion were evaluated through the simulation of the transition from island to step flow growth. The chemistry of GaCl and AICI was found to play an important role in the surface evolution. Finally, the linked kinetic Monte Carlo and the reactor scale models were used to study the morphology evolution as a function of the operating conditions. Based on our results we propose a mechanism underlying the morphology evolution of the A1GaAs, as films deposited by MOVPE systems.

9:45 PM T3.5
TIME DEPENDENT SURFACE MORPHOLOGY ASSOCIATED WITH GROWTH INTERRUPTS IN GaAs MOLECULAR BEAM EPITAXY. Anders Ballestad, Ben Rock, Jens Schmid, Tom Tiedje, Univ of British Columbia, Dept of Physics and Astronomy, Vancouver, BC, CANADA.

We have used ex-situ atomic force microscopy and in-situ elastic light scattering experiments to study the time evolution of the surface morphology of GaAs during growth by molecular beam epitaxy. Constant coefficient growth equations describe the surface evolution well during growth [1], but transient effects in the light scattering signal induced by growth interrupts indicate that the coefficients in the growth equation are flux and time dependent. The transition from a constant flux scenario towards a thermodynamical equilibrium on the surface, where islands and step edges settle into a more energetically favourable configuration, is proposed as an explanation for the decaying smoothing rate. We propose a mean-field rate equation approach in order to keep track of incorporation sites and adatoms on the surface during growth and post-anneal. The model extends beyond the dilute sub-monolayer description, and yields qualitative and quantitative agreement with our light scattering experiments. [1] Ballestad, Rock, Advancyck, Pinnington and Tiedje, Phys. Rev. Lett. 86, 2377-2380 (March 12, 2001).

10:00 PM T3.6
ATOMISTIC MODELING OF III/V SEMICONDUCTORS: THERMODYNAMIC EQUILIBRIUM AND GROWTH KINETICS. Frank Grobe,1,2 William Barvoine-Cavalcanti, Jean-Marc Zuck,3 Mark C. Gyure1, J. HRL Laboratories, LLC, Malibu, CA. 1Department of Mathematics, University of California, Los Angeles, CA. 2Department of Materials Science and Engineering, University of California, Los Angeles, CA.

The smaller the structural features of III/V semiconductor heterostructures, the more important the atomic nature of surfaces and interfaces. To utilize thermodynamical equilibrium and growth kinetics to design interfaces on the atomic scale makes detailed predictive modeling necessary. We describe a general method of III/V semiconductor modeling on the basis of ab initio density functional theory (DFT) calculations, supported by experimental results. Accuracy and predictability is evaluated using the example of a kinetic Monte Carlo (KMC) simulation for the InAs(001) surface. We present results for the phase transition between the \( \alpha_{2(2x4)} \) and \( \beta_{2(2x4)} \) reconstruction. Simulated island nucleation in the low coverage regime is in excellent agreement with experiment.

Furthermore, relevant microscopic processes for decrease of island number density and decrease of adatom density with increasing As pressure are revealed: Suppression of effective island density by incoming As leads to reduced island nucleation. This work is supported by NSF and DARPA through the Virtual Integrated Prototyping Initiative and the NSF Industrial Postdoc Program. The DFT calculations were carried out using the PHONON simulation package [1].

A phase-field theory of dislocation dynamics, strain hardening and hysteresis in ductile single crystals is developed. Specifically, we consider the motion of large numbers of dislocations within discrete slip planes through random arrays of point obstacles under the action of an applied shear stress. A statistical mechanical framework for dissipative systems was developed to include kinetic and thermal effects. The energy terms contemplated in the theory include the core energy of the dislocations, the long-range elastic interactions between dislocation segments, and the energy of interaction with the applied resolved shear stress. The simulation is carried out using a path integral Monte Carlo algorithm with an energy barrier due to the irreversible interaction between dislocations and point obstacles. The phase-field representation enables complex geometrical and topological transitions in the dislocation ensemble, including dislocation loop nucleation, bow-out, pinching, and the formation of Orowan loops. The theory predicts a range of behaviors which are in qualitative agreement with observation, including: hardening and dislocation multiplication in single slip under monotonic loading; softening at higher temperatures; Bauschinger effect under reverse loading; fading memory effect, whereby reverse yielding gradually eliminates the influence of previous loading; evolution of the dislocation density under cycling loading, leading to characteristic "butterfly" curves; and others. The theory permits the coupling between slip systems; the consideration of obstacles of varying strengths; and dislocation line-energy anisotropy.

CRUMPLED CANDY WRAPPERS AND BENT TAPE MEASURES.
Eric M. Kramer, Physics Dept., Simon's Rock College, Great Barrington, MA.

We discuss two topics related to the large-deflection behavior of thin-walled, elastic structures under compression. First, we review the mechanism of sound production from crumpled sheets of paper and plastic, and present recent results of high-resolution (200 kHz sample rate) digital recordings. Next we present a theoretical and experimental study of the V-shaped kink in a bent tape measure. Measurements were made of (1) the kink's longitudinal and transverse profiles and (2) the bending moment as a function of kink opening angle. Results show good agreement with the predictions of linear elasticity theory.

THE PHASE FIELD METHOD: MICROSTRUCTURAL EVOLUTIONS IN ALLOYS AND DISLOCATION DYNAMICS.

L. Freville, Y. Le Bouar, D. Rodney, A. Finel, ONERA, Chatillon, FRANCE.

The Phase Field Method has been extensively used to study the dynamical evolution of microstructures inherited from phase transformations. It has recently been extended to the dynamics of dislocations and thus to the domain of plastic deformation. We will present recent results in these two different fields. First, we analyze the competitive growth of different ordered precipitates in aluminum-based alloys (Al-Zn). Second, we present a recent extension of the Phase Field method to dislocation dynamics and plasticity. This new formalism incorporates simultaneously two different length scales, the first one associated to the dislocation core radius, and the second one, which is set by the discretization of the real space, associated to the long range scale of slowly varying concentration and long range order fields. This method will be illustrated of a first approach of alloy hardening.

RELATING ATOMISTIC GRAIN BOUNDARY SIMULATIONS RESULTS TO THE PHASE FIELD MODEL.
Catherine M. Bishop, W. Craig Carter, Massachusetts Institute of Technology, Dept. of Materials Science and Engineering, Cambridge, MA.

Atomistic simulations provide detailed results of grain boundary structures and energies in highly controlled numerical environments. Mesoscale models, such as the phase field model, are meant to extrapolate microscopic information—such as that calculated in an atomistic model, or measured from HREM—to a continuum and subsequently be applied to systems that are much larger and more complex than those that can be studied by direct simulation. We will present a method of coarse-graining information from atomistic simulations to order parameters that are required as the energetic basis of phase field models. The method extracts spatial information from sets of discrete data and yields a continuously variable order parameter that can be used to tune a phase field model.

COMPETITION BETWEEN NUCLEATION OF TWINS AND DISLOCATIONS: ATOMIC SIMULATION OF THEIR INITIATION DYNAMICS IN BCC-MOS.

Jinpeng Chang1, Eric M. Kramer, Dmitri E. Beresnev, Department of Chemical and Materials Science and Engineering, Rutgers University, Piscataway, NJ.

From finite-T MD simulations using a many-body interatomic potential, both twinning and dislocation are observed to form in perfect crystalline bcc-Mo in the aftermath of elastic instabilities driven by shear. In some cases the twin disappeared in continuing shear by twinning again in the original plane, while in others almost complete twin transformation achieved by the migration of jogged dislocation segments, and the energy of interaction with the applied resolved shear stress. The simulation is carried out using a path integral Monte Carlo algorithm with an energy barrier due to the irreversible interaction between dislocations and point obstacles. The phase-field representation enables complex geometrical and topological transitions in the dislocation ensemble, including dislocation loop nucleation, bow-out, pinching, and the formation of Orowan loops. The theory predicts a range of behaviors which are in qualitative agreement with observation, including: hardening and dislocation multiplication in single slip under monotonic loading, softening at higher temperatures; Bauschinger effect under reverse loading; fading memory effect, whereby reverse yielding gradually eliminates the influence of previous loading; evolution of the dislocation density under cycling loading, leading to characteristic "butterfly" curves; and others. The theory permits the coupling between slip systems; the consideration of obstacles of varying strengths; and dislocation line-energy anisotropy.

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We find not only competition but also cooperation in certain loading conditions, where the formation of twin domains facilitates nucleation of dislocations.

11:30 AM T4.0 SIMULATION OF ANELASTIC RELAXATION AND DEFECT INTERACTION IN ALUMINUM: Yoshiaki Kagawa, Toshio Kosugi and Masao Doyama, Tokyo University of Science & Technology, Yamanashi, JAPAN.

A large number of mechanical relaxation peaks have been observed in the temperature dependence of internal friction in metallic crystals. The point defects or defect complexes responsible to the peaks are interstitials, impurity pairs, impurity-interstitial pairs and so on. These defects accompany a non-spherical strain field and respond to the external shear stresses. The temperature dependence of internal friction and elastic modulus change are used to be analyzed on the basis of phenomenological anelasticity model developed by Norrie et al., in which the point defect strain per unit concentration is called as “the elastic dipole moment” and denoted by the A-tensor. According to the model the magnitude of relaxation is proportional to the square of A tensor. The relaxation time is the function of potential energy at a saddle point, and it can be calculated from the interaction potentials. Both the relaxation strength and the relaxation time for the point defects system in aluminum alloys are calculated in this study. The atomic displacement, the elastic field around the point defects, and the saddle point energy on the relaxation path are calculated by using the EAM potential based on the molecular dynamics simulation. The interaction of point defects through the strain field is very important. This improvement is mostly likely to lie in the break-up of the connectivety of random boundary networks. The experimental determination of the network topology has been accompanied by a microstructure modeling effort that is derived from the percolative nature of the network. The problem of point defect networks, under crystallographic constraint, has been simulated using a stochastic approach that considers the probability distribution function for each boundary based on the fluctuations in strain energy (from deformation) and intrinsic characteristics such as interfacial energy. The influence of both multiplicative and additive fluctuations toward microstructural evolution during recrystallization and grain growth will be elaborated. Experimentally derived measures to quantify microstructures such as in the grain boundary character and triple junction distributions will be compared to those obtained from simulations.

This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

11:45 AM T4.10 THE INFLUENCE OF MANY BODY INTERACTIONS IN THE STRESS VELOCITY RELATION FOR THE DEFORMATION IN A 2D LATTICE: M. Rehling, Centro de Investigacion en Energia UNAM, Priv. Xochicaleos S/N Col. Centro, Temixco, MEXICO; K. Kuksi and V. Muntone, Helsinki University of Technology, Laboratory of Computational Engineering, FINLAND.

The stress-velocity relation of one dislocation moving in a 2-D lattice has been studied using interactive molecular dynamic simulations. A hybrid model coupling the Lenard-Jones(LJ) potential and the Embedded Atom Model (EAM) potential is used to include radial and many body interactions. Both parts are assembled by a parameter that allows to change a pure radial interaction to a strong many body interaction in a continuous way. Setting up a constant-stress scenario, the movement of one dislocation is tracked from the rest, up to a terminal velocity state. The external stress vs. terminal velocity curves are obtained in a subzone regime for different values of the coupling parameter. Non-linear relations are found in 0.1c to 0.6c velocity range, where c is the transverse speed of sound. An analysis is done using an augmented Poiseuille Model to seek the connection between atomic scale, continuum variables and the limiting speed of dislocations.

T5: DEFORMATION-INDUCED STRUCTURES: STOCHASTIC METHODS

Tuesday Afternoon, November 27, 2001
Room 310 (Hyatt)
NOTE EARLY START

1:15 PM T5.1 STATISTICAL PROPERTIES OF DISLOCATION ASSEMBLIES: János Groma, Eötvös, Istan, HUNGARY.

It is well known that during the plastic deformation of crystalline materials the dislocation distribution does not remain homogeneous. In spite of the increasing experimental and theoretical activity on this field we are far from the understanding of this typically self-organizational phenomenon. A crucial open question is whether the long range dislocation-dislocation interactions which do not have an intrinsic length lead to spatial patterns which may exhibit well-defined characteristic scales. A possible approach for the modeling of these pattern formation processes is to investigate the collective behavior of systems consisting of individual dislocations by computer simulation. However, because of the long range character of the dislocation interaction the direct numerical integration of the equations of motion of dislocations is very computation expensive restricting considerable the affordable dislocation number or simulation volume. The aim of the investigations presented is to overcome this restriction by taking into account the statistical properties of the dislocation assembly. In order to describe the behavior of a system of straight parallel dislocations is investigated. This is a strong simplification of a dislocation network developing during plastic deformation, but it is an ideal model system for studying the consequences of long range interaction. It is found by numerical simulation that the stress vs. strain created by the dislocations has a stochastic component. In order to describe this stochastic character the form of the probability distribution function of the internal stress is determined. It is shown that the mean value of the distribution function is the self-consistent field created by the dislocation, and the distribution function decays with 1/r^2. On the basis of these analytical findings an O(N) stochastic simulation method is proposed. It is shown that the type dislocation pattern formation can be modeled by this approach.

1:45 PM T5.2 STOCHASTIC METHOD FOR THE EVOLUTION OF MICROSTRUCTURES WITH PARTICULAR REFERENCE TO GRAIN BOUNDARY NETWORKS: Roger W. Minich, Mahul Kumar, James S. Stilken, Christopher Schuh, Lawrence Livermore National Laboratory, Livermore, CA.

Grain boundary engineering has been successfully applied to improve materials properties such as intergranular corrosion and cracking, creep, weldability, and ductility. This has been attributed to an increase in the fraction of special grain boundaries resulting from theromechanical processing. Our investigations, however, have led us to conclude that the basis for these improvements is most likely to lie in the break-up of the connectivity of random boundary networks. The experimental determination of the network topology has been accompanied by a microstructure modeling effort that is derived from the percolative nature of the network. The problem of grain boundary networks, under crystallographic constraint, has been simulated using a stochastic approach that considers the probability distribution function for each boundary based on the fluctuations in strain energy (from deformation) and intrinsic characteristics such as interfacial energy. The influence of both multiplicative and additive fluctuations toward microstructural evolution during recrystallization and grain growth will be elaborated. Experimentally derived measures to quantify microstructures such as in the grain boundary character and triple junction distributions will be compared to those obtained from simulations.

This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

2:15 PM T5.3 TOWARDS A PHYSICAL THEORY OF CRYSTAL PLASTICITY: Anter El-Azab, Pacific Northwest National Laboratory, Richland, WA.

The motion of lattice dislocations induces plastic distortion of metallic crystals. Typically, dislocations are very large in number and their motion and interactions have a statistical character. Currently, the statistical aspects of a dislocation system are being probed using simulation models that are based on the fundamental aspects of individual dislocation lines interactions with the lattice stress field and among each other. Such computational models are statistically-mechanical in nature. Development of a formal non-equilibrium statistical mechanics framework however remains a challenge due to the significant fundamental differences between a dislocation system and a classical system of particles. Some recent progress along these lines is reported here. This progress has two basic ingredients. First, a new interpretation of the compatibility condition in a deforming crystal has been found, from which a new physical law has been extracted—a form of the integral of the dislocation density tensor over the reference crystal volume defines a topological invariant that characterizes a conserved quantity associated with the deformation field. Second, this invariance characteristic of this topological object is combined with the notion of phase space to develop a set of Louisville-type kinetic equations describing the transport and reactions of dislocations on all slab systems of a deforming crystal. Being linear topological objects, dislocations are modeled as a stochastic fiber process. The problem of crystal deformation is then treated as a holistic fashion where the elastic and plastic distortions and the deformation-induced dislocation and deformation patterns are potentially and simultaneously predictable.

2:30 PM T5.4 DISLOCATION PATTERNING IN TWO DIMENSIONS AND SIZE EFFECTS IN PLASTICITY: Robin L.B. Selinger, Brian B. Smith, Robin L. B. Selinger, Brian B. Smith, Eötvös, Istan, HUNGARY.

We study the dynamics of screw dislocations in two dimensions to characterize both defect patterning and size effects in plastic deformation. Our model is a close analogue of the XY rotor model under driving boundary conditions. In a homogeneous solid under a
constant shear strain rate, we observe spontaneous coalescence of screw dislocations into a pattern of slip bands. We also study deformation with temperature gradient geometry. In both cases we find clear differences in the effects of shear and of temperature scaling behavior. We discuss the origin of the size effect and the emergence of a characteristic length scale in plastic response.

The average disorientation angle increases with plastic strain differently for both types of boundaries in good agreement with experimental observations on different materials. An equivalent formulation as Fokker-Planck-equation for the distribution function of the disorientation angles allows the interpretation of the problem as diffusion (with or without drift) in a disorientation space with a distinct physical meaning of the diffusion coefficient. The resulting distribution functions show scaling behavior i.e. normalization of the disorientation angles by their average angle leads to a master distribution independent of strain, but depending on the degrees of freedom (number of dislocations sets in a boundary). Comparison with experimental data on cold-rolled aluminum shows a preference for a Rayleigh-distribution corresponding to two (dominating) independent dislocation sets in a boundary. An extension of the model allows the description of spatial correlations between the disorientation angles across neighboring boundaries. An anti-correlation arises from the limited free path of mobile dislocations before their trapping leading to a saturation of the disorientation angle across several boundaries. Experimental evidence is presented and opposing interpretations are discussed as well as the consequences on e.g. recovery.

Abnormal grain growth occurs when a small set of grains grow to consume all the other grains in the system. The phenomenon is of considerable industrial and academic interest but due to its stochastic nature it has been very difficult to study experimentally; the abnormal grains consuming all evidence of their origin. Computer models have advantage here, in that they can run time backwards to the initial point of an abnormal event. However there are various issues about studying and classifying rare stochastic events using a computer model, such as estimating the minimum size of the model that is required to yield a single event. In a system where the number of variables is very large defining the territory where these possible discrete catastrophic events might occur is very important. In this paper we describe our approach with a cellular automaton in which we gradually increases the complexity of the model in order map out the territory in which abnormal grain growth can occur. We compare our results with the geometrically based analytical theories and draw conclusions about the relative merits of the two approaches in predicting these sort of catastrophic events during microstructural evolution.

We present a kinetic Monte Carlo (kMC) simulation of the glide of a $<111>$ screw dislocation on the (011) plane in body centered cubic molybdenum in the presence of substitutional tantalum atoms. In the simulation, the dislocation is treated as a series of linear segments. The solute is distributed in 3-d while the dislocation is constrained to move in the glide plane via a kink mechanism. The kMC simulation include the elastic interactions between the dislocation and solutes as well as solute-core interactions. The model explicitly includes double kink nucleation, kink migration and kink-kink annihilation. In BCC molybdenum, kink migration is very fast compared with kink nucleation. This, together with line tension, tend to produce relatively straight screw segments. Thus, long times are required for the formation of a stable double kink. Before the dislocation migration simulations start, we pre-calculate the rate of nucleation of stable double kinks based on a stochastic model that includes elastic interactions, the applied stress, thermal fluctuations and the biased random walk nature of kink migration. In addition, the stable double kink nucleation rate also depends on the local solute distribution. The double kink nucleation model is shown to agree with analytical predictions in some simple limits. Incorporation of such a double kink nucleation model is a key to efficient simulations. Simulations are performed at several solute concentrations and a range of stresses. The stress-plastic strain rate relationships are determined by averaging over several simulations. The results are analyzed in terms of porocclusion theory.

In the presence of solutes, Chaitanya S. Deo, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI, Princeton Materials Institute, Princeton University, Princeton, NJ, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ; David J. Srolovitz, Princeton Materials Institute, Princeton University, Princeton, NJ, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ.

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This paper will summarize progress in our attempt to model the transport of dislocations through the partially ordered structures that are generated during deformation. The problem is characterized by strain bursts in time associated with the production of fine slip lines on the surface, and the spatial localization of the fine slip into growth bands. A percolation model previously developed applies to the fine slip features, but new approaches to what controls the time between bursts and mechanisms for the spatial localization will be presented. The time between percolation events is determined by recovery processes associated with cross glide and the nucleation of new events within a given slip band. The spatial localization is associated with the development of dense slip-termination walls parallel to the active slip plane which channel the slip. A feedback mechanism will be presented which stabilizes these walls in their open channel direction, while new channels are activated as strain increases by the nonpercolative activity.

SESSION T6: DEFORMATION-INDUCED STRUCTURES: CRACKS AND voids

Chair: Tom A. Asencio

Tuesday Evening, November 27, 2001
Room 310 (Hynes)

8:00 PM T6.1 BRANCHING IN BRITTLE FRACTURE. Leonard M. Sander, Jon Efroim, Michigan Center for Theoretical Physics, The University of Michigan, Ann Arbor, MI.

Many studies have confirmed that cracks in brittle materials branch when the crack speed exceeds a certain threshold, e.g., the value of this threshold is not understood. Almost all theoretical calculations overestimate it, by factors of two or more. We have shown (L.M. Sander and S.V. Ghaisas, "Thermal Noise And The Branching Threshold In Brittle Fracture" Phys. Rev. Lett. 85, 1994 - 1997 (1999); O. Pia, F. Guinec, E. Louis, S.V. Ghaisas and L.M. Sander, "Straight cracks in dynamic brittle fracture" Phys. Rev. E 61, 11472 (2000)) that thermal noise can reduce the threshold by a substantial amount, and we proposed that this effect can account for the discrepancy. In this talk we extend our treatment to account for quenched noise, and, again show that the threshold for branching is very sensitive to this effect.

8:30 PM T6.2 PHASE-FIELD MODEL OF MODE III DYNAMIC FRACTURE. Alain Karma, Dept. of Physics, Northeastern Univ., Boston, MA; David Kessler, Dept. of Physics, Bar-Ilan University, Ramat-Gan, ISRAEL; Herbert Levine, Dept. of Physics, Univ. of California, San Diego, La Jolla, CA.

We introduce a phenomenological continuum model for mode III dynamic fracture that is based on the phase-field methodology used extensively to model interfacial pattern formation. We couple a scalar field, which distinguishes between "broken" and "unbroken" states of the system, to the displacement field in a way that consistently coordinates the interactions between the two. Almost all theoretical calculations overestimate the value of the threshold for coalescence, by factors of two or more. We have shown (L.M. Sander and S.V. Ghaisas, "Thermal Noise And The Branching Threshold In Brittle Fracture" Phys. Rev. Lett. 85, 1994 - 1997 (1999); O. Pia, F. Guinec, E. Louis, S.V. Ghaisas and L.M. Sander, "Straight cracks in dynamic brittle fracture" Phys. Rev. E 61, 11472 (2000)) that thermal noise can reduce the threshold by a substantial amount, and we proposed that this effect can account for the discrepancy. In this talk we extend our treatment to account for quenched noise, and, again show that the threshold for branching is very sensitive to this effect.

9:00 PM T6.3 MODELING VOID NUCLEATION IN COPPER BY ULTRA-SHORT PULSE, LASER-DRIVEN SPHERICAL SHOCKS. J.S. Stolken, M.-J. Caturla, B.A. Remington, Lawrence Livermore National Laboratory, Livermore, CA.

The performance of materials under short time scales and high pressures applied through laser interactions is of great interest for the development of targets for inertial confinement fusion applications. Shock propagation has traditionally been studied using continuum models. However, under certain conditions and geometries the boundary conditions applied to the problem can have an impact in the solutions obtained. Such a situation arises when studying spherical shocks, in particular, at the convergence point. One way of overcoming this limitation and understanding the effect of converging shock waves is to use molecular dynamics simulations. We have studied with this method the effect of spherical shocks on a copper target. The pulse width applied was 1 ps, with peak stresses between 1 and 20GPa. The initial condition is a copper sphere 35nm in diameter. The embedded atom method was used as the interatomic potential for this simulation. We observe the propagation of the shock through the target, and follow its change in character (compression vs. tension) and structure. As a result of the applied deformation a void is generated at the center of the copper sphere. We analyze the formation of the void with respect to the type and strength of the shock applied. We correlate the size of the void with the peak stresses, the size of the original system, and compare to known scaling relations.

This work was carried out under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under contract W-7405-Eng-48.

9:15 PM T6.4 ATOMICISTIC STUDIES OF THE STRUCTURAL MODIFICATIONS IN FUSED SILICA DUE TO SHOCK COMPRESSION. Miriam A. Bureau, M. Davila, J. S. Stolken, S. Sadigh, A. Quong, A. M. Rubenchik and M. D. Feit, Lawrence Livermore National Laboratory, Livermore, CA.

We have studied the atomic-scale processes of dynamic shock-loading of fused silica using molecular dynamics simulations. The calculations predict macroscopic properties such as shock velocity, shock pressure and densification, which are in agreement with experiments. In addition, detailed analysis of the microstructure shows structural modifications associated with permanent densification. An increase in the number of 3- and 4-membered rings is observed after shock densification in agreement with Ramses measurements. Changes in coordination of silicon and oxygen atoms are also observed, related to the formation of defects. We discuss the structural modifications in terms of ring, coordination, defect and void spatial distributions. These simulations explain some of the underlying mechanisms in high-power laser damage, where a shock wave is expected to develop. Moreover, they can provide quantitative measurements of changes in the strength of the material during dynamic transformation. Parameters such as density changes or viscosity could then be used as input for macroscopic models of damage. In particular, the obscuration and damage growth during continuous irradiation of these materials will depend on the interaction of the modified silica glass with the laser beam. Therefore, the optical properties of this modified silica must be studied. We have computed, using first principle methods, the electronic and optical properties of some of the defects formed during shock-loading. These defects were identified in the classical molecular dynamics simulations mentioned above.

This work was carried out under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under contract W-7405-Eng-48.

9:30 PM T6.5 STRUCTURAL-PHASE TRANSFORMATIONS IN THIN FILM Ni₃Al-TAKING PLACE AT THE PRESENCE OF THE CRACK-INITIATOR IN THE DEPENDENCE ON TEMPERATURE AND PRESSURE. M.S. Dmitriev, A.A. Ovcharov, G.M. Poletayev, D.M. Starostenkov, General Physics Department, Altai State Technical University, Barnaul, RUSSIA.

Structural-phase transformations in two-dimensional thin film of intermetallic Ni₃Al, taking place in a zone of the crack-initiators in the dependence on deformation, temperature and time are investigated. The interactions between Ni-Al are given by the pair interatomic potentials of Morse type. This film is presented by the packing of the plain [111] of FCC lattice. The crack-initiator is oriented in the direction <112>. Structural-phase transformations in the system are investigated by the method of the molecular dynamics. The distribution of velocities of the atomic displacements in the dependence on temperature is given according Boltzman statistics. At the expense of the atomic diffusion of alloy components, the development of the crack is accompanied by the appearance of the phase germs of Ni₃Al and Al composition. The kinetics of the reaction is regulated by the temperature and the value of applying pressure. The velocities of similar transformations are determined. The zones of segregations of Al and Ni atoms in the head of the crack-initiators are found. The dislocation mechanisms, regulating the development of the crack according the mechanism of transformation from brittle behavior to plastic one are defined. The presence of germs of new phases also influences on the dynamic of the crack growth.

SESSION T7: LIQUIDS, GLASSES, AND SOLID-LIQUID INTERFACES

Chairs: Brian D. Wirth and Susan N. Coppernsmith

Wednesday Morning, November 28, 2001
Room 310 (Hynes)

8:30 AM T7.1 STATISTICAL MECHANICS TOOLS FOR NON-EQUILIBRIUM LIQUIDS. Denis J. Evans, Research School of Chemistry, Australian National University, Canberra, ACT, AUSTRALIA.

We summarize recent developments in the field of non-equilibrium molecular dynamics (NEMD) computer simulations of fluids.
Developments include: the "method of planes" methods for computing the spatial variation of thermodynamic and transport properties within narrow pores, and the use of entirely configurational information to estimate the temperature. The latter permits us to estimate the local temperature of systems undergoing complex, possibly time dependent flow. We also describe new methods that allow us to control the temperature of systems using entirely configurational, as opposed to kinetic, methods.

9:00 AM T7.2
ATOMIC-SCALE MODELING OF HETERO PHASE INTERFACES IN A\(Al\)\(2\)\(O\)\(3\) and Si\(O\)\(2\) Systems, A. van de Walle, Dept. of Materials Science and Engineering, Northwestern University, Evanston, IL; J. Hoyt, Sandia National Laboratories, Albuquerque, NM; A. Karma, Northeastern University, Boston, MA.

Static and dynamic properties of heterophase interfaces play a critical role in dictating non-equilibrium structural evolution resulting from phase transformations. Quantitative modeling of phase transformation microstructures requires a detailed understanding of such interface properties which are characteristically difficult to extract directly from experimental measurement. We will describe the application of classical atomic-scale simulation methods to the study of thermodynamic and kinetic properties of heterophase interfaces in alloys. We focus on applications to alloy solidification where the morphology of dendritic microstructure is sensitively influenced by the degree of crystalline anisotropy in solid-liquid interface properties. Simulations are based upon classical many-body potentials of the embedded-atom formalism where alloy cross-interaction terms are derived from reduced-order principles for total-energy calculations. Static properties of solid-liquid interfaces in alloys are derived through Monte-Carlo simulations which provide equilibrated structures as input to molecular dynamics simulations. Due to the rapid time scales associated with liquid-phase diffusion and atom attachment/detachment kinetics at rough solid-liquid interfaces in metals, large-amplitude molecular dynamics simulations can be applied directly to the calculation of equilibrium and non-equilibrium properties of solid-liquid interfaces including (anisotropic) excess free energies, interfacial mobilities and non-equilibrium partitioning. This work is supported by the U.S. Department of Energy through the Computational Materials Science Network and the Office of Basic Energy Sciences.

9:30 AM T7.3
THERMODYNAMIC PROPERTIES OF SOLID-LIQUID INTERFACES FROM ATOMICISTIC SIMULATIONS, J. Hoyt, Sandia National Laboratories, Albuquerque, NM; M. Asta, Dept. of MSE, Northwestern University, Evanston, IL; A. Karma, Physics Dept., Northeastern University, Boston, MA.

It is well known that during the solidification of alloys, the shape and velocity of a growing dendrite depends critically on the anisotropy of the solid-liquid interfacial free energy, \(\gamma\). We demonstrate that this small anisotropy can be computed from molecular dynamics simulations by monitoring the statistical fluctuations in the height of the interface. Results are reported for Ag, Au, Cu, Ni and Pb where the methodology is used to describe the interatomic potential. In addition, it will be shown how the interfacial stress, the excess energy and the excess entropy of the solid-liquid boundary can be obtained from atomistic simulations. In particular, the excess entropy can be computed in two ways, from separate computations of both the excess energy and \(\gamma\) or from a direct calculation of the thermodynamic potential of the interfacial free energy. Results of the two methods will be compared and the values of the excess entropy will be discussed in terms of existing statistical mechanics models.

10:30 AM T7.4
AN EXTENDED CAHN-HILLIARD MODEL FOR INTERFACES WITH CUBIC ANISOTROPY, Theyathar Ahmedandeh, Indian Institute of Science, Bangalore, INDIA; Ferdinand Haider, Univ. Augsburg, GERMANY.

For studying systems with a cubic anisotropy in interfacial energy \(\sigma\), we extend the Cahn-Hilliard model by including in it a fourth rank term, \(1/2\mu(\nabla\nabla \phi)^2\), to an additional linear term in the evolution equation forth composition variable. This also leads to an orientation-dependent effective fourth rank coefficient \(\mu\), where \(\phi\) is the governing equation for the one-dimensional composition profile across a planar interface. The main effect of a non-negative \(\mu\) is to increase both \(\sigma\) and interfacial width \(w\), each of which is related to \(\mu\) through a universal scaling function. In this model, \(\mu\) is a differentiable function of interface orientation \(\phi\), and does not exhibit cusps; therefore, the equilibrium morphology of the Wulff shapes (Wulff shapes) do not contain planar facets. However, the anisotropy in the interfacial energy can be large enough to give rise to corners in the Wulff shape in two dimensions. In particles of finite sizes, the corners get rounded, and their shapes tend towards the Wulff shape with increasing particle size. Using this model, we studied the influence of an anisotropic interfacial energy on dendritic solidification.

10:45 AM T7.5
SIMULATION OF CRYSTAL-MELT INTERFACES FOR A SYSTEM OF BINARY HARD SPHERES, Rachel Silug Aga and Brian B. Laird, Univ of Kansas, Dept of Chemistry, Lawrence, KS.

Crystal-melt interfaces of binary hard spheres are investigated using molecular-dynamics simulation. The system, which is a simple model for binary alloys, consists of a two-component fluid of hard spheres of differing size (defined by the diameter ratio \(a\)), in equilibrium with the coexisting crystal phase. For a diameter ratio of \(a = 0.414\), two crystal phases coexist with the fluid phase in contact with the pressure. At low pressures, the liquid coexists with a pure fcc crystal of the larger particle, while at high pressures a 1:1 binary crystal of "NaCl" type is the coexisting phase [Tricca, et al., Mol. Phys. 90, 675 (1997)]. For both of these systems, we study the structure and dynamics in the interfacial region as functions of interface orientation. In particular, it is observed that as the interface moves from fluid to crystal the diffusion constant of the larger particle vanishes before that of the small particle defining a region of the interface where the large particles are frozen in their crystal lattice, but the small particles exhibit significant mobility. This behavior was not observed for binary hard spheres with diameter ratio of 0.9 [Davidchack and Laird, Mol. Phys. 97, 833 (1999)]. In addition, structural and dynamical relaxation across the interface do not occur over the same region. Traversing the system from the crystal side to the fluid side, structural relaxation is seen to occur first.

11:00 AM T7.6
SIMULATION OF STRESS RESPONSE AND MECHANICAL RELAXATION IN METALLIC GLASSES, Yoshihiko Kogure, Masao Doyama, Teikyo Univ of Science & Tech, Yamanashi, JAPAN.

Materials of the glassy state, a quenched state of liquid, are known to show peculiar mechanical properties, which is related to the disordered configuration of atoms. Elastic and anelastic responses to the external stresses are investigated by calculating the displacement and the relaxation of atoms under the stress based on the molecular dynamics simulation. Metallic glasses of binary alloy, such as Ag-Cu and Ag-Ni, are chosen as model systems. The simulation systems of these two materials contain several thousands of atoms and the periodic boundary condition is adopted. Embedded atom method potentials for the materials developed by the present authors are adopted. The structure of the systems in glassy states is examined through the radial distribution function. The external stress is applied by deforming the simulation cell, and the motion of atom is monitored. The distribution of internal stress is evaluated from the configuration of the nearest neighbor atoms and the potential energy of individual atoms. The relaxation of internal stress is monitored. Especially a large relaxation is observed under the shear stress. The crystallization from the amorphous state is one of the useful process to produce a nanophase material. The amorphous state of the model system is also tried to realize the partial crystallization, and the changes of atomic structure in the system are investigated.

11:15 AM T7.7
TRANSPORT PROPERTIES OF LIQUID AND AMORPHOUS METALLIC SYSTEMS USING MOLECULAR DYNAMICS TECHNIQUES, Frank J. Cherng, Michael I. Baskes, Los Alamos Natl Laboratory, Los Alamos, NM; Pierre A. Deymier, University of Arizona, Dept of Materials Science and Engineering, Tucson, AZ.

The advanced casting modeler requires accurate viscosity and diffusivity data of liquid metals and their alloys. The general scarcity of this data combined with the experimental difficulties in obtaining such data motivates this work. Utilizing both the equilibrium and non-equilibrium molecular dynamics techniques, we calculate the diffusivity and viscosity of several technologically important metals and their alloys (i.e. aluminum, nickel, zirconium, aluminum-nickel alloys, and nickel-zirconium alloys). We compare the transport properties obtained from both EAM and MEAM potentials to the available experimental data. The results from this work indicate that equilibrium and non-equilibrium molecular dynamics techniques provide reliable and accurate data required by the advanced casting modeler.

11:30 AM T7.8
SIMPLE ATOMIC MODEL WITH UNUSUAL THERMODYNAMIC PROPERTIES FOR A SYSTEM OF BINARY HARD SPHERES, Rachel Silug Aga and Brian B. Laird, Univ of Kansas, Dept of Chemistry, Lawrence, KS.
Using molecular dynamics simulations we studied the thermodynamic behavior of a recently proposed model of a single-component covalent material with atomic interactions described by an empirical environment-dependent interatomic potential (EDIP). The model exhibits a range of unusual properties typically found in more complex materials. They include negative thermal expansion coefficients for the crystalline and low-temperature amorphous structures, and the existence of two structurally distinct disordered phases. Structural differences between the two disordered phases lead to a first-order transition between them and imply the existence of a second critical point. Such behavior is analogous to that believed to exist for amorphous forms of frozen water. This research was supported by the NSF grand DMR-0074273.

11:45 AM T8.7
"PSEUDO-ChARGE-TRANSFER" SIMULATION METHOD FOR LIQUID AMORPHOUS AND METALLIC SYSTEMS.

Frank J. Chere, Ricardo B. Schwartz, Michael I. Baskes, Los Alamos National Laboratory, MST-8, Los Alamos, NM; Pierre A. Deymier, University of Arizona, Dept. of Materials Science and Engineering, Tucson, AZ; Srivijithurup G. Srinivasan, Los Alamos National Laboratory, T-11, Los Alamos, NM.

Molecular dynamics has proven a useful tool for understanding the structure of liquids and glassy structures. Although these simulations predict non-equilibrium properties of the amorphous melts, they fail to reproduce more detailed changes in properties with composition (i.e., radial distribution functions, viscosity, and shear modulus). It has been shown that current potentials used to simulate metals predict certain structural information for the binary alloy vastly different from experiment. The limitations of these simulations may be related to the fact that potential models used to describe short-range interactions often neglect the role of charge transfer between the elements. A strong charge transfer is expected between pairs of elements with large negative heats of mixing. We have incorporated charge transfer effects in our potentials using two methodologies: by a direct evaluation of Coulombic charge transfer and by changing the atomic radius of an atom depending on its atomic environment. We will present the results for two binary metallic systems with rich phase diagrams, namely, aluminum-nickel and nickel-strontium. These model systems were chosen primarily due to the complexity of their phase diagrams. For the first alloy we are interested in reproducing the value and composition dependence of the liquid viscosity, whereas in the second alloy we are interested in reproducing the measured changes in the shear modulus with composition in its amorphous phase. It will be shown through an analysis of a variety of properties that each of these "pseudo-charge-transfer" techniques can provide valuable insights into the structure and formation of metallic glasses.

SESSION T8: INTERFACES IN POLYCRYSTALS AND ALLOYS

Chairs: Sidney Redner and Jeffrey J. Hoyt
Wednesday Afternoon, November 28, 2001
Room 310 (Hynes)

1:30 PM T8.8.1 GRAIN BOUNDARY AND DISLOCATION MIGRATION IN ALLOYS.

David J. Scalapino, James E. Mendelev, Chaltanya S. Deo, Princeton Materials Institute and Dept. of Mechanical & Aerospace Engr, Princeton University, Princeton, NJ.

The motion of extended defects, such as grain boundaries and dislocations, in crystalline materials generally occurs by nucleation and propagation of kinks on one-dimensional defects and islands on two-dimensional defects. Models for defect motion based upon this mechanism have been studied for decades. In this presentation, we discuss the motion of extended defects in crystalline materials in the presence of solute. Solute atoms can have both long-range and short-range interactions with extended defects. In most cases, it is the short-range interactions that have the largest effect on defect migration. We present a series of simulation studies based on generalized Ising models that examine the influence of static and diffuse impurities on the motion of extended defects. In particular, we focus on the cases of grain boundaries, where the impurity interactions are short-range only and on dislocations where there are both long- and short-range interactions. We also present the g Gerry models for the mobility of these defects as a function of solute concentration, solute diffusivity and the heat of solute segregation.

2:00 PM T8.2 MONTE-CARLO STUDIES OF ORDERING KINETICS IN THE LONG-PERIOD SUPERLATTICE ALLOY Co-Pd-X. Wang, K.F. Ludwig Jr., Boston University, Dept. of Physics, Boston, MA; X. Flamant, R. Caudron, ONERA, Chatillon, FRANCE.

Monte-Carlo studies of the 1-d long-period superlattice (LPS) ordering kinetics in Cu-Pd have been performed at the 21 at. Pd composition. Long-range effective pair interaction potentials for the simulations were derived from x-ray diffuse scattering experiments. The simulations reproduce the equilibrium LPS structure of the alloy as well as the salient kinetics features observed in our time-resolved x-ray scattering studies. The important kinetic phenomena observed include a delayed growth of the central superlattice peaks relative to the satellite peaks and a nonmonotonic evolution of the satellite peak positions with time. The simulations show that, following a quench of the disordered alloy into the 1-d LPS region of the phase diagram, compact structures first form that are modulated in more than one direction. Both conservative and non-conservative antiphase boundaries are initially present. Only later do these compact modulated regions grow anisotropically, eliminating the nonconservative antiphase boundaries, and forming the equilibrium 1-d modulated LPS structure. This work has been partially supported by NSF DMR 9633596.

2:15 PM T8.3 MICROSTRUCTURE EVOLUTION IN ELASTIC MATERIALS UNDERGOING STRUCTURAL TRANSFORMATIONS.

Tubur Lookman, Avadh Saxena, Subodh Shenoy and Dorothy Hatch, Theoretical Div, Los Alamos Natl Lab, Los Alamos, NM.

We show how a unified understanding of both displacive and reconstructive phase transformations is possible from a mesoscopic Ginzburg-Landau free energy entirely in strain variables. An important feature is a long-range anisotropic interaction in the order parameter whose shape couples different elastic textures under various thermodynamic conditions. For instance, local stress inhomogeneities can affect structures on a global scale. The formalism is readily applied to all major crystal systems in 2D and 3D. We will illustrate it for structural transformations of the square and triangular lattices in 2D. We present microstructure results of dynamic simulations relevant for materials such as Fe-Pd and lead-orthovanadate.

2:30 PM T8.4 ATOMICALLY-BASED CONTINUUM FORMULATION FOR DIFFUSIONAL PHASE TRANSFORMATIONS.

Krishna Garikipati, Univ of Michigan, Dept. of Mechanical Engr, Ann Arbor, MI.

Diffusional transformations in crystalline materials are modelled. A continuum formulation is developed, that nevertheless accounts for the atomic-level processes of exchange, agglomeration, generation and annihilation of species. Such mechanisms are considered, and, accompanied by local states of stress and strain, provide the thermodynamic basis for this approach. Densest internal energy, work and entropy are thus constructed explicitly and combined into the Gibbs free energy density. Formal methods of continuum mechanics then yield constitutive equations that reflect the coupling of composition and mechanics. Balance laws, consisting of continuity equations coupled between diffusing species and the equation of quasistatic stress equilibrium, complete the continuum description. This formalism has been previously been applied to stress-assisted self-diffusion in polycrystalline metals. The addition of surface/interface energies, composition-dependent properties, nucleation conditions and mechanically and physically-motivated methods for interface evolution will be discussed. These will allow the modelling of diffusional phase transformations that follow the kinetics of nucleation-and-growth or spinodal decomposition.

Applications of interest include phase precipitation and clustering during dopant diffusion—a stage in semiconductor manufacture, and strain-based self-assembly of micro/nano-structures. Void nucleation in metal interconnect lines, due to self diffusion of metal atoms mediated by stress and electric fields, has many features in common with problems of phase transformation and can be formally treated using these methods. The spatial scales involved in these processes are in the micron to deep submicron range, motivating the atomically-based methods. The theory and formulation will be discussed with special emphasis upon the aspects that are crucial to diffusional phase transformations. Some special solutions will be demonstrated and, time permitting, numerical implementation and examples will be presented.

2:45 PM T8.5 COMPUTATIONAL EVALUATION OF THE PHASE DIAGRAM OF THE Au-Ni BINARY ALLOY.

Determination of the Solvus, Liquidus, and Solidus lines as predicted by an EAM POTENTIAL. E. Ogando1, M. Cars2, and A. Cars3, 1Electrica eta Elektronika S拆, UPV-EHU 644 P.K., Bilbo, SPAIN; 2Centro Atomico Bariloche, Bariloche, ARGENTINA; 3Atomic Simulation Group, Queen’s University Belfast, NORTHERN IRELAND, UNITED KINGDOM.
Dynamical Self-Organization under Irradiation of Alloys Undergoing Phase Separation and Ordering

Jiwen Liu, Pascal Bellon, Materials Research Laboratory, University of Illinois at Urbana-Champaign, IL.

Experiments on Ni-Al have suggested long ago that, under appropriate conditions, ion irradiation can induce a stable coexistence at a finite, nanometer scale of a chemically ordered phase (here an L12 ordered phase) with an fcc solid solution (A1 phase). However, the origin of such a mesoscopic phase coexistence, as well as the wavelength selection rules, has remained so far unclear. For the simpler case of an alloy exhibiting a miscibility gap between two disordered solid solutions (e.g., Cu-Ag), recent theoretical and simulation work indicates that spontaneous organization can be due to the irradiation forced atomic jumps take place at a finite range in displacement cascades, whereas thermally activated diffusion proceeds by short range jumps. In the present work, we extend this approach and we consider the case of an alloy that can both undergo phase separation and phase ordering. We introduce a time-dependent Ginzburg-Landau model that describes the evolution of the alloy under irradiation. Various models are discussed for the forced mixing: short range, finite range, or arbitrary range mixing. Atomistic kinetic Monte Carlo simulations, using a vacancy-based mechanism for thermal diffusion and various forced mixing models, are performed on an fcc lattice and compared to experiments. A linear stability analysis of the continuum model indicates that for moderate irradiation-induced jump frequency, the alloy may self-organize into patterns of coexisting L12 and A1 phases. This self-organization is driven by the impact of the finite range forced mixing on the composition field. This prediction is confirmed by our kinetic Monte Carlo simulations: under moderate irradiation conditions phase coexistence of L12 ordered phase and A1 disordered phase saturates at the nanometer. These results corroborate the idea that irradiation can be used as a method to synthesize nanocomposite materials containing chemically ordered phases.

Phase Transformations Induced by Arsenic Implants Into Silicon

James P. Levine, David D. Tuschel, Donald L. Black, Eastman Kodak Company, Rochester, NY.

Micro-Raman spectroscopic investigations of arsenic-implanted silicon show lines characteristic of silicon crystallites [1] even at implant doses above the amorphization threshold. The intensity and frequency of occurrence of the lines increase with the implanted dose. The present polarization/orientation Raman studies rule out silicon in the diamond phase as the source of the 505 to 510 cm\(^{-1}\) line and indicate the 520 cm\(^{-1}\) optical phonon line is not due to the substrate silicon. Monte Carlo simulations of the arsenic ion energy loss suggest each arsenic ion deposits sufficient energy to locally melt the silicon lattice. This is supported by detailed molecular dynamics calculations for low energy implants [2], which find the localized heating dissipates in picoseconds. It is probable that upon cooling a phase transformation leads to silicon crystallites in both the diamond phase (Si-I) and the hexagonal phase (Si-IV), as the observed Raman lines are consistent with these phases. Hexagonal silicon was found by Tan et al. in diffraction studies of arsenic-implanted silicon [3]. This work will briefly outline the Raman spectroscopic evidence for the two phases of silicon. This will be followed by a careful examination of the time scales for heat dissipation and arsenic ion cascade overlap. Simple estimates for the former based on the thermal diffusivity of silicon lead to nanoseconds, while the latter factor brings in dose effects. These time scales are important for estimates of the crystallite size resulting from the phase transformations. The energetics of the formation of Si-IV versus Si-I will also be addressed.

Motion of Boundaries by Discretized Mean Curvature in 2D and 3D Spin Models

Elizabeth A. Holm, Materials and Process Modeling, Sandia National Laboratories, Albuquerque, NM, Mark A. Miodownik, Department of Mechanical Engineering, King's College London, London, UNITED KINGDOM.

Spin models, such as kinetic Monte Carlo Ising and Potts models, are statistical mechanics models widely used to study grain growth, Ostwald ripening, magnetic domain coarsening, and other phenomena driven by surface energy minimization. However, the relationship between motion of a discretized boundary and motion of a continuum
boundary has not been elucidated. We show that under appropriate conditions, a discretized boundary moves with velocity proportional to its discretized mean curvature. Thus, boundaries in spin models obey a discrete version of the continuum boundary motion law. The presence of domain junctions and lattice anisotropy also influence boundary motion in spin model systems.

4:45 PM T9.11 CURVATURE DRIVEN GRAIN BOUNDARY MIGRATION IN ISING MODEL. Mikhail I. Mendelev, David J. Srolovitz, Princeton Materials Institute and Dept. of Mechanical & Aerospace Eng., Princeton University, Princeton, NJ.

The evolution of polycrystalline microstructures is determined by the relative ease with which grain boundaries can move. The boundary mobility is the ratio of the boundary velocity and the driving force for migration. In order to test whether the mobility of the boundary is independent of the type of driving force and the migration geometry, we have performed a series of simulations within the framework of a simple, Ising model. In particular, we simulate boundary migration on a 2-D triangle lattice with non-conserved spin and Glauber dynamics. Two types of boundary motion are considered: motion under an applied driving force (magnetic field) and curvature driven grain boundary migration. In the first case, we consider boundary motion in two distinct crystallographic directions. It is found that the mobilities for these two direction of motion are not only different in magnitude but exhibit fundamentally different temperature dependences. The mobility of the boundary with an applied driving force can be satisfactorily described using a kink model. Curvature driven boundary migration is examined in both half-loop and circular grain geometries. The mobility is found to depend only very weakly on the half-loop orientation. While the boundary mobilities were very similar for all angle of motion, the motion is driven by temperature, they are much different than those found in the presence of an externally applied force. The mobilities measured in the curvature driven cases were found to be much weaker function of temperature than those found in the presence of an applied force. The shape of the half-loop is in excellent agreement with an analytical, continuum model.

SESSION T9: DISORDERED MATERIALS
Chair: Babak Sadigh
Wednesday Evening, November 28, 2001
Room 310 (Hynes)

8:00 PM T9.1 HOW LONG DOES IT TAKE FOR A FILTER TO CLOG? Sidney Redner, Boston Univ, Dept of Physics, Boston, MA.

In depth filtration, a dirty fluid is "cleaned" by trapping dirt particles within the pore space during flow through a porous medium. These trapped particles block individual pores until the filter is clogged and no additional flow occurs. This leads to a self-generated gradient percolation process which exhibits a power-law distribution for the density of pores at a constant distance from the input. A deterministic model for the pore space is introduced which predicts the trapped particle distribution. The time evolution of the clogging process is also studied. The most interesting situation is when the particle and pore size distributions overlap substantially. By developing a simple extremal model for the history of the clogging process, we find that the mobility of the boundary changes as the boundary moves from a free to a pinned state. The results of this model are in excellent agreement with simulations of filtration on lattice networks. Some consequences of this model for optimal filter operation are also discussed.

8:30 PM T9.2 MIXING PHASE FIELD AND FLUID-STRUCTURE INTERACTIONS. Adam Powell, David Dussault, MIT, Dept of Materials Science and Engineering, Cambridge, MA.

A phase field model is presented for transport of elastic solids in a fluid, using a reduced elastic-viscous stress formulation. Elastic modulus is set to zero in the fluid, and viscosity to zero in the solid, with intermediate values of both in the diffuse interface. The model has been validated against single-Cahn-Hilliard free energy functional, but extension to more complex free energies is straightforward, including anisotropic functions where local orientation is updated according to the vorticity. An illustration of the model using finite differences in two dimensions is presented. Numerical difficulties such as interface erosion are discussed.

5:45 PM T9.5 ACTIVATED FRONT PROPAGATION IN RANDOM MEDIA. Rune Skoe, Damien Vandembroucq and Stéphane Roux, Unité Mixte CNRS/Saint-Geobain Aubervilliers, FRANCE.

We present a numerical study of the propagation of an elastic chain in a random pinning potential at finite temperature. Depending on the range of the elastic interaction this model can describe vortex motion in type II superconductors, charge density waves in solids, wetting or crack front propagation. We focus on the velocity-force characteristics and the front roughness statistics on the creep regime in type II superconductors, charge density waves in solids, wetting or crack front propagation. We present a numerical study of the propagation of an elastic chain in a random pinning potential at finite temperature. Depending on the range of the elastic interaction this model can describe vortex motion in type II superconductors, charge density waves in solids, wetting or crack front propagation. We focus on the velocity-force characteristics and the front roughness statistics on the creep regime.
The work was performed in part 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.


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 talk, we present a model of cluster growth and deposition processes based on a combination of Direct Simulation Monte Carlo (DSMC) and Monte Carlo (MC) methods introduced to examine the effects of temperature and conditions on cluster expansion 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.


10:30 AM T10.6 SIMULATION OF VAPOR DEPOSITION AND POSTANNEALING OF AMORPHOUS NANOSTRUCTURES. V.M. Burlakov, A.P. Sutton, G.A.D. Briggs, Department of Materials, University of Oxford, UNITED KINGDOM; Y. Tsukahara Technical Research Institute, Toppan Printing Co Ltd., JAPAN.

A recently developed model for the defect network structures [1] is used in these simulations of vapor deposition and annealing of the amorphous Si, C, SiOx, and SiO2-Si-O-Si nanostuctures. The problem of the pore formation in amorphous Si and SiOx is studied in detail. The model predicts that Si grains can be more disordered but less porous than those deposited quasistatically. Their subsequent annealing results in an increase of porosity, and the pore formation/growth is driven by the decrease in the total energy of topological defects (oxygen and silicon dangling bonds). Comparing a set of SiO2 and Si structures simulated under similar conditions, including a hypothetical 3-fold coordinated Si shows that the ultimate porosity is determined by the effective atomic coordination number, bond-bending force constant, and the dangling bond energies. Simulated annealing of the SiO2-Si-O-Si nanostuctures reveals a tendency toward crystallization within the amorphous Si layer, in accordance with the experimentally observed formation of nanocrystallites in thin Si layers confined in silicon. The model is extended onto situation of vapor deposition and postdeposition of amorphous carbon.


10:45 AM T10.7 MODIFIED LANGEVIN THERMOSTAT FOR CONSTANT TEMPERATURE - CONSTANT PRESSURE MD SIMULATIONS OF POLYMER SYSTEMS. A. Caro², J. Kohanoff², and M. Finnis¹.

¹Centro Atómico Bariloche - Instituto Balseiro, Bariloche, ARGENTINA. ²Atomic Simulation Group, Queen's University Belfast, N. Ireland, UNITED KINGDOM.

The Parinello-Rahman algorithm is one of the standard algorithms for molecular-dynamics (MD) simulations of periodic systems. Its strategy is based on the incorporation of the degrees of freedom of the simulation box (both size and shape) as additional dynamical variables, which evolve according to the resultant of the external and internal stresses. For finite non-periodic systems, like small clusters, a recent paper by Martonak et al. [1] proposes a model version of the actual experimental procedure, i.e. the use of a fluid as a conveyor of the thermal and pressure external variables. This fluid, modeled by a simple pair potential interaction with known equation of state (T,P) undergoes collisions with the atoms in the cluster as a consequence of the simultaneous integration of the equations of motion of the cluster and fluid particles. This algorithm simulates the way pressures are applied to clusters in real experiments and does not represent an increase of the computational effort if the number of particles in the fluid is small, or if the equations of motion of the larger atoms form expensive ab-initio total energies. Weaknesses of this approach are: (1) the number of particles in the fluid can not be too small if they are to be considered as a T-P reservoir, and (2) equilibration of the fluid is necessary prior to the physical contact with the system under study. In this work we present a new algorithm based on a different approach. Atoms in a cluster come to thermal equilibrium through interaction with a surrounding degree of freedom that carry information about the T-P conditions. However, the description of the collision process with these degrees of freedom does not need the integration of their equations of motion. The bath is characterized by a well-defined distribution of kinetic variables, which is the only relevant physical information for the cluster. These degrees of freedom are equivalent to the hypothesis of Brownian motion as described by stochastic Langevin equations. In these equations, random forces represent the collision with the ambient medium and are related to the bath which is characterized by a well-defined distribution of kinetic variables. These degrees of freedom are equivalent to the hypothesis of Brownian motion as described by stochastic Langevin equations. In these equations, random forces represent the collision with the ambient medium and are related to the bath which is characterized by a well-defined distribution of kinetic variables. These degrees of freedom are equivalent to the hypothesis of Brownian motion as described by stochastic Langevin equations. 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certain text format (called UDF; User Definable Format). The GUI program controls any simulation programs and can analyze simulation results by using the Python language. New programs can be easily incorporated into the OCTA system by using the UDF text format. This work is supported by the national project, which has been entrusted to the Japan Chemical Innovation Institute (JCII) by the New Energy and Industrial Technology Development Organization (NEDO) under METI's Program for the Scientific Technology Development for Industries that Creates New Industries.

11:30 AM *T10.10
GOING THROUGH ROUGH TIMES: FROM NON-EQUILIBRIUM SURFACE GROWTH TO ALGORITHMIC SCALABILITY.
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Modeling and simulation of the evolution of natural and artificial complex systems are of fundamental importance in both science and engineering. In a large class of systems the underlying dynamic is inherently asynchronous. Examples of such systems include magnetization dynamics in condensed matter, cellular communication networks, and the spread of epidemics. Constructing a parallel scheme for simulating the time evolution of these systems, in which the local changes in the configuration are asynchronous, leads to at least two difficult questions. First, to put it simply, "How to design parallel algorithms for non-parallel dynamics?". Second, if there is a faithful parallel algorithm for the problem, "Is it scalable?". We describe novel parallel Monte Carlo algorithms for asynchronous systems with both the computation and the measurement part being asymptotically scalable. In particular, we discuss the intimate connection [1] between algorithmic scalability and non-equilibrium surface growth phenomena, which has led us to the engineering and fine-tuning of fully scalable massively parallel schemes.

Supported by NSF, NERSC-DOE, CSIT-FSU, MSU, and RPI.