SYMPOSIUM KK

KK: Atomic Scale Materials Design-Modeling and Simulation

December 1 - 4, 2003

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*Invited paper
8:30 AM *KK1.1 Chemical Realism in Chemo-Mechanical Processes For Multi-scale Models, Rodney Hunge, Marshall Cory and Peter Rontowy, Quantum Theory Project, University of Florida, Gainesville, Florida.

Simulations can only be as accurate as are the forces provided to the MD. For yet many problems, including all bond breaking processes and optical properties, we require a fully quantum mechanical treatment of the forces. *Ab initio* correlated, electronic structure theory like coupled cluster theory is predict to within small error bars for most properties of molecules of 18-20 atoms. DFT can extend this predictability to maybe 100’s of atoms in some cases. But neither can provide forces quickly enough for large scale MD simulations. Using aspects of coupled-cluster theory, we show that there is a quantity we call the transfer Hamiltonian that can account for the quantum mechanical treatment of the forces; and these can be obtained with sufficient efficiency that they can be tied to MD in direct dynamics mode. The transfer Hamiltonian is chosen to be of the NDDO form common to semi-empirical quantum chemistry, but its atomic parameters are obtained via a genetic algorithm to ensure that the forces are the same as those of *ab initio* methods for representative clusters. Since the form of Hamiltonian is short-range, the atomic parameters saturate with the cluster size leaving a size-independent, converged form of Hamiltonian. All calculations are done fully self-consistently and are quantum size specific in that they account for different dispersion paths like radicals versus ions. We illustrate the application of the transfer Hamiltonian to chemo-mechanical processes by considering the fracture of silicon in the presence of water and other examples. This work is supported by the NSF under grant DMR-0925593.

9:00 AM KKL.2 Evaluation of mechanical response of smectic interlayers during hydration using steering molecular dynamics, Dinesh R. Katti, Steven Schmidt, Pijush Ghosh and Kalpana Katti, Civil Engineering, North Dakota State University, Fargo, North Dakota.

Smectic clays are materials of importance in geotechnical and geoenvironmental engineering and in the field of clay-polymer nanocomposites. These minerals exhibit large swelling and exert swelling pressure in interaction with fluids. Understanding the interaction between clay and water or other fluids is important for the proper use of these materials. In this work the mineral structure of a model system, pyrophylite is used to construct a model of the mineral montmorillonite through hygroscopic inorganic substitutions. The response of the interlayer is evaluated using molecular dynamics simulations. Steered molecular dynamics simulations are conducted. Forces are applied to the surface (bound oxygen) to evaluate the displacement of the applied pressure in the interlayer and hence the swelling pressure between two clay layers at atomic scale. Swelling response is measured for single and double layers of water. The simulations indicate that under applied compressive stresses of 0.165 GPa, the maximum deformation of the interlayer is almost linear. The predominant deformation of the clay model results from deformation of interlayer spacing. Deformation of the clay layers observed in this stress range, although not insignificant, is small. Further, at low stresses (0.2 GPa), as the clay layers approach each other, the non-bonded interlayer forces are dominant over the mechanical applied forces. However, as the stresses increase the mechanical forces overcome this effect and the interlayer spacing decreases linearly. In addition, compressive response of individual components, the clay layer and interlayer at are found. This work gives insights into the molecular interface between clay and solvent molecules under externally applied loads. The paper describes the construction of the model, the simulation procedure, and results of steered molecular dynamics simulations obtained.

9:15 AM KKL.3 Simulation Studies of Size Effects in Plastic Deformation, Robin Selinger, Brian B. Smith and Scott Weigarten; Physics, Catholic Univ., Washington, District of Columbia.

In order to study size effects in plastic deformation, we perform atomistic simulation studies of deformation of a polycrystal in a strain-gradient geometry. The polycrystal’s initial grain structure is generated via the models described in the paper. The samples are confined between parallel walls whose radii of curvature gradually decrease with time, producing an applied bending strain. Mechanical response is measured via a generalized bending moment as a function of strain. We examine yield mechanisms as a function of temperature and look for evidence of size effects in plastic response. These results are compared with mesoscale simulations of size effects in plastic deformation. Using an idealized model of screw dislocations in two dimensions, we model anti-plane plastic deformation in a strain gradient geometry and characterize the resulting size effects.

Mechanical response of the interior of the sample is consistent with the Bingham plastic law, while the boundary region exhibits an anomalously hard plastic response. We explain why the Bingham plastic law breaks down near the boundary where dislocation image interactions strongly reduce the local dislocation density, and examine factors determining the thickness of the anomalous plastic layer. We discuss implications for understanding size effects in plastic deformation.


Void growth and coalescence are known to be important ductile fracture mechanisms in metals. Under shock conditions, such as those encountered in explosively loaded materials, the attendant high deformation rates may induce the formation of small layers characterized by a large concentration of nano and microvoids arranged in spatial patterns. The diffusion, growth and coalescence of these voids can lead to material failure under typical experimental conditions. Therefore, a detailed understanding of the main mechanisms by which these voids grow and interact is required in order to construct reliable multiscale models of spallation in metals. Recently, molecular dynamics (MD) simulations have revealed the nucleation of large dislocation loops in Cu and Al. However, the size constraints inherent to MD make it difficult to obtain a complete picture of the relevant mechanisms. In this paper, we employ the quasicontinuum method (QC) in order to study voids and samples of realistic size under meaningful deformation conditions. In QC the continuum and atomistic scales are seamlessly bridged, thereby enabling information at the atomistic scale where required, yet allowing a coarse-grained description of the material where the magnitude of the deformation is small. Results showing the nucleation and transport of dislocation loops are presented for fcc metals such as Al and Cu.

9:45 AM KKL.5 Dislocation Glide in Model Ni(Al) Solid Solutions by Molecular Dynamics, Georges p. Martin1, Erwan Rodrey2, David Rodrey2 and Yves Brechet2, 1CEA, Chenay-Mahboy, France; 2INP, Grenoble.

The glide of an edge dislocation in an EAM random solid solution: Ni (1 to 8% Al), is simulated by molecular dynamics. The EAM potential has been optimized to reproduce correctly the relevant properties of the face centered cubic solid solution of the L12 Ni3Al phase. Glide is studied at fixed temperature and applied stress. Three parameters, Sr, B and Sd, are found necessary to describe the rate of shear for a given applied shear stress. Sr is the static threshold stress, below which the glide distance of the dislocation is not sufficient to insure sustained shearing. Sd is the dynamical threshold stress, which reflects the friction of the pinning potential on the moving dislocation. B is the friction coefficient which relates the effective stress (Sr+Sd) to the glide velocity. Sr and B increase linearly with the solute content. In the viscous regime, the glide of the dislocation segment is described by a simple "stop and go" model. A random population of obstacles with a distribution of waiting times is assumed to oppose the glide of the dislocation segment. Detailed analysis of the trajectory of the latter yields the mean obstacle density and the distribution of waiting times, as a function of stress and composition. The values found for the mean waiting time per obstacle suggest that the unlocking of glide proceeds by the collective motion of few (3 to 5) atoms. The obstacles are argued to be made of configurations of the large Al atoms which are brought in positions of strong mutual repulsion in course of glide. The glide-Coble-Orowan short range repulsion, rather than the direct dislocation-solute interaction, is thus argued to be the mechanism mainly responsible for chemical hardening. A simple way for taking advantage of the above results in the frame of multiscale modeling is exemplified.

10:30 AM KKL.6 Multiscale Modeling of Fracture: Combined Cohesive Models and First Principles Calculations, Santiago Serebrinsky1, Emily A Carter2 and Michael Ortiz2, 1Graduate Aeronautical Laboratories, California Institute of Technology, Pasadena, California; 2Department of Chemistry and Biochemistry, University of California Los Angeles, Los Angeles, California.

Cohesive theories of fracture have been a recourse to obtain fracture properties of materials under several conditions. Application of the method to analyze the effect of different constraints usually required
 calibration to fit experimental data for specific samples. In this way, a successful description of some fracture features has been achieved. In this work, we present a new approach to the construction to determine fracture properties. We propose a method to coarse grain an initic calculation of material properties that allows for the computation of fracture properties at the macroscopic level by means of bulk calculations. The coarse division of the structure is accomplished by a series of calculations to fracture. The method involves several steps linked in succession, viz., a) calculation of atomistic cohesive laws by first principles (e.g., density-functional theory), b) renormalization of the cohesive laws for many particles in the stress process, c) elastic correction to avoid double counting of elastic properties, and d) embedding of the renormalized law into a finite element calculation with cohesive elements. A detailed description of each step is presented. Actual and prospective applications of the method, including hydrogen embrittlement and stress corrosion cracking, are discussed in terms of microscopic as well as macroscopic variables. The results obtained so far are highly promising.

Hybrid Quantum-Classical Dynamics Simulation of Water Enriched Perovskite: a Case Study

Shuji Ogna1, Tatsuro Kurosawa2, Kiyota Aji, Akihiko Igarashi2, 3

Japan Science and Technology Corporation, Kyoto, Japan.

In recent years, there has been much development in the hybrid quantum-mechanical/molecular-dynamics (QM/MD) schemes for multi-scale simulation of materials. In our hybrid schemes, a QM region composed of a small number (less than a few hundreds) of atoms is treated with the density-functional theory based on a large scale MD system. In the present simulation, we employ the hybrid simulation methods that consist of a QM region and a classical region. We perform detailed investigations on the mechanical properties and the effects of hybridization on electronic structures of the QM region. We apply the present scheme to the stress corrosion cracking of both Si and aluminium systems by environmental water and hydroxyl molecules, to understand its microscopic mechanisms. In the case of Si, the hybrid simulation results show that the reaction of water molecules at a silicon crack tip is sensitive to the stress intensity factor K. For a relatively small value of K, a water molecule either decomposes and adheres to the crack surfaces or oxidizes Si, resulting in the formation of a Si-O-Si structure.

11:45 AM KKL 1.8
Hybrid scheme between large-scale electronic structure methods and its application to fracture simulation

Takao Hosho, Ryu Takayanagi1, Tatsuro Igarashi2

1Department of Applied Physics, University of Tokyo, Hongo, Bunkyo-ku, Tokyo, Japan.
2Japan Science and Technology Corporation, Tokyo, Japan.

A hybrid scheme between large-scale electronic structure methods is developed and applied to fracture simulation of silicon with up to more than 100,000 atoms using a standard single-CPU work station. We have developed several order-N methods as large-scale electronic structure methods. The order-N method is the name of electronic structure calculations, in which the computational cost is proportional to the system size. We have developed the (i) variational and (ii) perturbative order-N methods with generalized Wannier states (J. Phys. Soc. Jpn, vol. 69, No.12, p.3773-3776 [2000]). We also use (iii) the recursion method and (iv) the exact diagonalization method. Practical calculations were done using transferable tight-binding Hamiltonians. Now we construct a hybrid scheme between the above methods. The hybrid scheme is advantageous to large-scale, fully quantum mechanical calculations, because the above methods are different in the accuracy, computational cost, and for applicability. The hybrid scheme is formulated by dividing the occupied Hilbert space into two parts: one is the space of reliable electronic structure calculations and the other is constructed from several occupied wave functions. Such subsystems are orthogonal with each other. Each subsystem is obtained with a mapped Hamiltonian under the conditions of the other. The mapped Hamiltonian is well defined in quantum mechanics, each subsystem can be solved by any quantum mechanical method, such as the diagonalization and order-N methods. In result, different subsystems are solved by different methods, which is the present hybrid scheme. These calculations are done by the combination of the diagonalization and perturbative methods, 2) the variational and perturbative methods, 3) the recursion and perturbative methods. Several test calculations are also done with parallel computers. The hybrid scheme is applied to molecule dynamics simulation in the fracture of nanocrystalline silicon with up to 100,000 atoms (cond-mat/0210580 v3). Dynamical fracture processes are simulated under external loads in the [001] direction. The hybrid scheme is done by the combination of the density-functional theory based on the localized Wannier states. Wannier states are solved by the perturbative method in the bulk region, in which the Wannier states are kept constant during the stress simulation. On the other hand, Wannier states are solved by the variational method near the fractured region, where some of the Wannier states change their character drastically from the sp3 bonding state into surface ones. We observe the formation of new surfaces and surface reconstruction processes. The element analysis is carried out with a quantum mechanical viewpoint. Step formations are also observed in larger samples. Several related calculations are also done.

11:15 AM KKL 1.9
Hybrid Electronic-Density-Functional/Molecular-Dynamics Scheme for Multi-scale Simulations of Semiconductors

Shuji Ogna1, Tatsuro Kurosawa2, and Tatsuro Igarashi2

1Nagoya Institute of Technology, Nagoya, Aichi, Japan.
2Japan Science and Technology Corporation, Kyoto, Japan.

In recent years, there has been much development in the hybrid quantum-mechanical/molecular-dynamics (QM/MD) schemes for multi-scale simulation of materials. In our hybrid schemes, a QM region composed of a small number (less than a few hundreds) of atoms is treated with the density-functional theory based on a large scale MD system. In the present scheme, we employ the hybrid simulation methods that consist of a QM region and a classical region. We perform detailed investigations on the mechanical coupling between the QM and MD regions and the effects of hybridization on electronic structures of the QM region. We apply the present scheme to the stress corrosion cracking of both Si and aluminium systems by environmental water and hydroxyl molecules, to understand its microscopic mechanisms. In the case of Si, the hybrid simulation results show that the reaction of water molecules at a silicon crack tip is sensitive to the stress intensity factor K. For a relatively small value of K, a water molecule either decomposes and adheres to the crack surface or oxidizes Si, resulting in the formation of a Si-O-Si structure.

11:30 AM KKL 1.10
Atomistic simulation of the interaction between a microcrack and hard inclusions in β-SiC: Alessandro Mazzoldi1, Luciano Colombo2 and Fabrizio Cleri3

1INFN and Department of Physics, University of Cagliari, Monserrato (CA), Italy.
2Unita` di Materiali e Nuove Tecnologie, ENEA, Roma.

Silicon carbide is a relevant structural material employed for the fabrication of components. In these compounds the SiC matrix is reinforced by hard fibers, usually made of carbon or carbon-coated SiC. Microcracks in such a composite can propagate within the matrix and should be arrested or deflected by the hard inclusions. The overall effect of the hard fibers is to increase the toughness of the material fracture work with respect to the bare matrix. We study the interaction of cracks induced by local stresses and the strain field of an elliptical microcrack in crystallographic SiC by means of atomistic large-scale molecular dynamics simulations. The interaction between Si and C atoms is described by a Tersoff empirical model potential. Constrained crack propagation is employed to represent the external load in plane strain approximation. The three-dimensional microcrack geometry is represented by a two dimensional section of the crack borders in the two directions perpendicular to that of the applied load. Hard inclusions, which are meant to describe the effect of reinforced fibers, are represented by model sections of graphite- and diamond-like carbon surrounding the microcrack with different densities and geometrical arrangement. The size of the inclusions is always comparable to that of the microcrack. The configurations containing inclusions are annealed at low temperature and relaxed at T = 1 K. The resulting interface between matrix and inclusions can be
either perfectly coherent and under tensile stress, or disordered, thereby reducing the interfacial stress. The static perturbation induced on the nanocrystals is characterized by mapping the stress and strain fields of the microcrack with and without the inclusions. Effects due to the non-additivity of the perturbations from the individual inclusions are elucidated by plotting differences between the respective stress and strain fields. The influence on the stability of the microcrack in presence of hard inclusions is characterized by studying the variation in the Griffith critical load as a function of density and geometry of the hard inclusions.

11:45 AM KK1.11

**Lattice Trapping Barriers To Brittle Fracture In Silicon**

Nanocrystalline Polycrystals and D. W. Hess, Center for Computational Materials Science, Naval Research Laboratory, Washington, District of Columbia.

Simulations of fracture in silicon, a prototype brittle material, have the potential to give insight into fundamental properties that control the behavior of the material at the crack tip. We show that in many empirical potentials there is a large energy barrier to brittle fracture caused by the discrete nature of the atomic lattice. In some cases the barrier is large enough to completely suppress brittle fracture, explaining the ductile behavior seen in many simulations. In contrast, a multimode simulation method that dynamically couples a quantum-mechanical tight-binding description of bonding at the crack tip to a larger empirical-potential simulation shows brittle fracture with only minimal lattice trapping, in agreement with experiment. A simple model for the interplay between the energy to break the crack tip bond and for energy relaxation correctly predicts the barrier for both the empirical-potential and coupled simulations. The success of the model indicates that the bond breaking process is highly local, and that deviations from linear elasticity at the crack tip are essential for determining the onset of lattice trapping. Two length scales emerge from the model: one for bond breaking, and another for elastic relaxation. Finally, we present ongoing work on dynamically coupled simulations for the fracture process in silicon at high temperatures, and fracture in other materials.

**SESSION KK2: Electronic Materials and Properties**

**Chair:** Norman Bernstein

Monday Afternoon, December 1, 2003

Constitution A (Sheraton)

1:30 PM **KK2.1**

**Atomic Scale Studies of High-k Gate Dielectrics**

Kyongjoo Cho, Gyungchun Jun, Seonghee Huh, Shirin Ramazanir, David Chi, Saunne Steemers, and Paul C. McIntyre, 1Department of Mechanical Engineering, Stanford University, Stanford, California; 2Department of Materials Science & Engineering, Stanford University, Stanford, California; 3Department of Materials, University of California-Santa Barbara, Santa Barbara, California.

Future gate dielectrics in CMOS devices will scale to sub-0.5 nm equivalent oxide thickness (EOT). At these dimensions, alternative oxides with higher dielectric constants (κ) than SiO2 will be required. To date, the different properties and thin films are not understood. High-k oxides are often comprised of complex, a-proti unknown multiple layers resulting from film growth reactions. Interdiffusion, nano-chemistry, phase separation, and crystallization. Such complex structures make a fundamental understanding of defects and interfaces and their relationship to MOSFET properties difficult. In this talk, we will discuss our current atomic scale studies of high-k gate dielectric materials with emphasis on the different composition using experimental and theoretical characterization methods. First, we will present the results of density functional theory (DFT) calculation to study the atomic and electronic structures of various layers of silicon and thin film layers. The influence on the stability of the hexagonal thin films subjected to high-temperature annealing. The oxygen K-edge fine-structures can be interpreted as an overlap of features from amorphous silicon and crystalline silicon phases in the phase separated microstructures. We also describe the use of deposited H2O/SiOx nano-crystals to probe the kinetics of phase separation in this binary system. The comparative analysis between theory and experiment elucidates the atomic scale structures and kinetic behaviors leading to a qualitative understanding of High-k dielectric materials properties. Acknowledgement: This research is supported by SRC contract 1015-001. We also acknowledge many helpful discussions with TI high-k research group (Luigi Colombo and Shuming Tang).

2:00 PM **KK2.2**

**Electronic-structure calculations of Nitrogen and Hydrogen in diamond twist grain boundaries.** Michael Sternberg, 1 Peter Zopoli, 2 and Larry A. Curtiss, 1, 2 1Materials Science Div., Argonne National Laboratory, Argonne, Illinois; 2Chemistry Div., Argonne National Laboratory, Argonne, Illinois.

Diamond films with grain sizes of 3 to 10 nm grown in methane/argon plasma show an increase of several orders of magnitude in n-type conductivity upon nitrogen addition to the plasma [Bhatt et al, Appl. Phys. Lett. 70, 1441 (2002)]. Our previous experimental studies have shown that nitrogen impurities are more stable in the grain boundaries than in the bulk. Using a density-functional-based tight-binding method, we have investigated the atomic and electronic structure of \( \Sigma 13 \) and \( \Sigma 29(100) \) diamond twist grain boundaries containing hydrogen and nitrogen at the same time. We have studied the formation of N–H complexes and associated changes in the electronic structure of the film for different hydrogen to nitrogen concentration ratios. We have also calculated participation ratios in order to find mobility edges in these systems and investigate the formation of defect/all-hydrogen bonds in the forbidden gap of diamond. These studies are used to understand the experimentally observed changes in the electronic properties of the films associated with changes in the plasma composition during the growth process.

2:15 PM **KK2.3**

**Stability of High-Energy Grain Boundaries in Nanocrystalline Si and SiC: Parallel MD, Tight-Binding MD, and Hybrid Tight-Binding/Classical MD Studies.** Kenji Tasumi, 1 Chieko Totsuji, 1 Hiroo Totsuji, 1 and Shige Ogata, 2 1Electrical & Electronic Engineering, Okayama University, Okayama, Japan; 2Systems Engineering, Nagoya Institute of Technology, Nagoya, Japan.

Classical and tight-binding (TB) molecular-dynamics (MD) simulations are performed to study thermal stability of some typical high-energy grain boundaries in nanocrystalline silicon and silicon carbide. We find that the thickness of amorphous-like grain boundaries in Si is independent of interatomic potential, stress values, and initial setup of the simulations. Thermal stability of SiC grain boundaries, on the other hand, quite sensitive to local bonding characters, i.e. presence/absence of Si-Si and C-C bonds at each grain boundaries. We also employ a hybrid TB/MD (classical MD) method to investigate stress and tractions of nanocrystalline Si and SiC. The behavior of impurities such as hydrogen atoms at these grain boundaries are analyzed by the method. (Work supported by ACT-JST and Grant-in-Aid for Young Scientists (B) No. 14760564 by MEXT.)

2:30 PM **KK2.4**

A critical re-address of silicon self-diffusion based on temperature-accelerated tight-binding molecular dynamics. M. Cugoni, 1 Luciano Colombo, 2, F. Montalenti, 2 B. Uhlenings, 3 and A. Voter, 2 1INFN and Department of Physics, University of Cagliari, Monserrato (CA), Italy; 2INFN and Department of Materials Science, University of Milano-Bicocca, Milano, Italy; 3Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico.

Many fundamental materials properties (e.g. microstructure evolution under processing, mass transport, bulk thermodynamics) are ruled by the diffusion of native point defects (self-diffusion). We developed a new approach using a thorough quantum mechanical picture - based on tightly-binding molecular dynamics (TBMD) simulations - of silicon self-diffusion has been presented, that is both consistent with state-of-the-art experimental data and able to predict separately the vacancy and self-interstitial (dumbbell) contributions [Jasso and others, Phys. Rev. B vol 64, p. 233203 (2001)]. We have extended the above investigation by developing for the first time a quantum (tight-binding) simulation scheme in the framework of the novel temperature-accelerated dynamics (TAD) method [Voter and others, Annu. Rev. Mater. Res. vol 32, p. 231 (2002)]. TAD-TBMD simulations have provided a more comprehensive picture on self-diffusion, especially in the case of self-interstitials. In particular, new pathways for dumbbell migration have been pointed out, suggesting that a rich hierarchy of diffusivity mechanisms (differing in migration energies and prefactors) should be indeed admitted. In this work we report the theoretical implementation of the present TAD-TBMD scheme and we critically re-address the self-diffusion phenomena in crystalline silicon.

2:45 PM **KK2.5**

**Diffusion of oxygen in silicon quantum chemical simulations.** Vasili E. Guskov and Leonid I. Mura; Inst. of Solid State and Semiconductor Physics, Minsk, Belarus.

In the present work the results of quantum-chemical simulation of diffusion of interstitial oxygen atom (O\(_i\)) in silicon and influence of uniform pressure upon the value of a diffusion barrier are presented. It is shown, that in the elementary diffusion act nearest Si atoms
are involved and the value of a diffusion barrier is determined by an
optimum configuration of these silicon atoms. For the first time both
the prefactor for the diffusion barrier and the barrier height have
been evaluated and are in excellent agreement with experimental results: \( \Delta E_{\text{diff}} = 2.59 \text{ eV} \),
\( \Delta E_{\text{diff}} = 0.3 \text{ cm}^2 \text{ s}^{-1} \) and \( \Delta E_{\text{diff}} = 2.59 \pm 0.56 \text{ eV} \). Using this model, the total energy released is
described by the following expression \( \Delta E_{\text{diff}}(P)/\Delta E_{\text{diff}}(P = 0) = 1 - 1.69 \times 10^{-3} \text{ kJ} \). We have found that the calculated pressure
dependence of the diffusion barrier value well describes an increase in the
oxygen thermal donors formation rate observed experimentally in Si-
hemitrodes under homogeneous pressure.

3:30 PM KK2.6
Rapid Crystallization of Si-B and Si-Ge Alloys. Erik J. Albers
and Paullette Clancy. School of Chemical and Biomedical
Engineering, Cornell University, Ithaca, New York.

Technological solutions are being sought to reduce unwanted boron
diffusion in ultra-thin source/drain regions in advanced electronic
devices. One approach involves the use of pulsed lasers in the
nanosecond or microsecond regime to ameliorate post-implantation
materials in order to induce crystallization and repair implantation
damage. One such approach involves employing explosive
crystallization to ameliorate damage in boron-doped silicon or SiGe
alloys. In this paper, the explosive crystallization of Si-B and
Si-Ge alloys has been studied using a non-equilibrium Molecular
Dynamics simulation method and a Stillinger-Weber potential model.
We have shown recently that this computational approach is capable of
emulating explosive crystallization, giving rise to a high speed process
which is converted to crystal facilitated by a mediating liquid layer. The drive force behind this
reaction is the enthalpy of fusion and the difference in melting
temperatures between the two solid phases (crystalline and amorphous).
We experimentally investigated the dependence of the boron doping level and Ge
concentration on the speed of the ensuing explosive crystallization
process and the structure of the resultant material. In the case of the
Si-B and Si-Ge alloys, the results show that the growth front velocity does not scale
linearly with composition, in agreement with experimental
results, despite the apparent conformity of the alloy's constituents.
For the case of boron-doped silicon, we focus on the ability of
explosive crystallization to prevent transient enhanced diffusion.

3:45 PM KK2.7
Defect Structures in Tin-doped and Tin-Zinc Co-doped
Indium Oxide Transparent Conductors. Donald E. Ellis,
Oscar Wachtler, Mitulch Lohmar and Jason A. Seuse, Physics and
Astrophysics, Northwestern University, Evanston, Illinois.

Tin-doped and tin-zinc codoped indium oxide (ITO and ZITO) are
transparent conducting oxides with many applications in areas such as
display technology, solar panels, opto-electronic devices etc. The
electrical properties of these materials are critically dependent on Sn
and In doping levels and the applied oxygen partial pressure during
deposition. Further, the details of the underlying defect chemistry as
an atomistic scale remain poorly understood. We report results using
an empirical atomistic model and focus in particular on the binding
energy of interstitial and structural oxygen in the In_{2}O_{3} lattice. This
binding energy is calculated through a local optimization of Sn
and In cation defects. We propose that the ability of ITO and ZITO to form n-type
conductors upon reduction is directly related to the amount of
loosely bound, and thus reducible oxygen in the lattice. In ITO, n-type
conductors are produced through reduction of interstitial oxygen
carbons which change balance Sn-dopants. The reducibility of interstitial oxygen
however is strongly influenced by the number of nearby Sn
dopants leading to increased binding at high Sn-doping levels. This
explains the experimentally observed decay in carrier concentration
at medium to high tin-doping level. In ZITO, our calculations indicate
that structural oxygen atoms in the vicinity of zinc dopants become
less strongly bound, with increased local environment leading to
increased conductivity compared to non-doped In_{2}O_{3}.

4:00 PM KK2.8
First-principles investigations of N-V-O complexes in Si.
Hiroaki Kageyama1, Akito Taguchi1 and Kazumi Wada2
1NTT Basic Research Labs., NTT Corp., Atsugi, Kanagawa, Japan;
2Massachusetts Institute of Technology, Cambridge, Massachusetts.

Nitrogen (N) doping in Si has received keen attention because it
significantly reduces the concentrations of both defects and dislocation
loops. To obtain high quality Cauchy-scale-grown silicon, control of
vacancy (V) aggregation and oxygen (O) precipitation are the two key
factors. It is experimentally obvious that the N doping suppresses V
aggregation and affects the formation of O precipitates. Although the
N doping effect on V aggregation has been theoretically investigated,
the effect on O aggregation has not been theoretically investigated.
In this paper, we report the formation of coupled complexes of N, V, and
O investigated by using the first-principles calculations. Since our
previous investigations of the N-doping effect showed that N forms various
stable complexes of both interstitial and substitutional type,
\((N\{V\}) + O \rightarrow (N\{V\}O)\). As widely accepted, an O atom is
assumed to occupy the bond center (BC) site when isolated. We
considered various possible sites of O around \((N\{V\})\), and then
computed the total energies for lattice relaxation to examine the
stable configuration. Our calculations found that \((N\{V\})O\) and O forms several
stable complexes. In the most stable complex, an O atom locates the
second nearest neighbor site of an N atom. The O atom moves to the
atom on the plane made by the \((N\{V\}) O\) complex, perhaps reducing the
strain. The energy benefit in the formation of this complex is as large
as 0.95 eV. Therefore, the \((N\{V\}) O\) complex effectively captures an O
atom during growth. Our investigation together with enhanced
oxygen precipitation observed experimentally is strongly suggestive that
the complexes would act as the oxide nucleation sites.
Thermodynamical properties of the complexes will also be discussed
to make clear the O agglomeration processes.

4:15 PM KK2.9
First-principles investigation of point defects in cubic silicon
carbonitride, Sabina Bernardini, Andrea Manganelli and
Niccolo Colombi, INFN and Dept. of Physics, University of Cagliari,
Monserrato, Italy.

Silicon carbide is a very promising material for semiconductors
device applications which have to work under extreme conditions.
Yet, the application of SiC in real devices have been hampered
because of the difficulties to grow high quality material. Both
extended and point defects in as-grown, interstitials and vacancies are
present in sizeable concentration in silicon carbide. Native defects in
SiC have been occasionally studied theoretically both by first
principles and semi-empirical methods. A widespread overview on the
structure and electronic properties found formation energy and defects
in SiC based on large cell calculations is still missing. Such
an investigation is important per se and as a preliminary work to allow a
reliable parameterization of semi-empirical methods like the tight-binding.
In this work we performed a systematic investigation of point defects in SiC
using present state-of-the-art first principles computational methods. We find that the carbon vacancy is the
most dominant defect in p-type SiC. For Si and C antisites are the
most common defect in the nitride material. Interstitial defects are
less favorable from the energetic point of view with respect to vacancies
and antisites. Likewise pure silicon, the dumbbell structure is the
lowest-energy configuration for the self-interstitial defects.

4:30 PM KK2.10
Multi-Scale Investigation of Molecular Oxygen
Decomposition and Incorporation into Si(100)-(2x1) Surface.
Alain Esteve1, Nicolas Richard2, Ansar Alimeshanoud3 and Melodi
Djafari Rouhani3,1; 3LAAS CNRS, Toulouse, France; 2DCRE,
CEA-DAM, Bruguiere le Chatel, France; 3Laboratoire de Physique des
Solides, Toulouse, France.

The silicon/silicon dioxide interface displays the most remarkable
properties of all semiconductor/oxide interfaces of the microelectronics
industry. Despite a considerable research effort in both experimental
and theoretical domains to push the technology to nanometer scales, little is known about its growth mechanism: oxygen
decomposition, incorporation into silicon and subsequent structuring of
the interface is poorly understood and still subject to controversy.
Nevertheless, this knowledge becomes crucial to any process modelling
tool for ultimate SiO2 technologies including emerging high-k
materials where intermediate SiO2 is invariably formed at the
Silicon/Silicon dioxide interface. Recently, STM and Infrared advanced
codensation techniques [1,2] have demonstrated new insight into
the atomic scale understanding of the early stage of silicon oxidation.
In particular, precise atomistic configuration are derived from the experimental data that enlighten the dissociation phenomena
and explain the presence of the stable transition state to the reactive
oxygen migration. We present first principle calculations of molecular
oxygen interaction with silicon Si(100)-(2x1) surface aimed at
reproducing the experimental picture and at completing the
calculating the theoretical one [3]. Non dissociative and dissociative chemisorption are
discussed as a function of the surface morphology and chemistry.
Further oxygen incorporation into Si-Si bonds, migration,
agglomeration and associated energy barriers are investigated in
detail. We finally show how these results are extrapolated to build a
Kinetic Monte Carlo procedure enabling direct oxidation process
simulation. This multiscale approach provides a unique opportunity to
link the past experiments with the ab initio level to rationalizing the advantages of both methods taken separately. Preliminary results
are presented in that direction. [1] Y.J. Chabal, K. Raghavachari, X.
4:45 PM KK2.11
Simulation Tool for Metal-Organic Vapor Phase Epitaxy of III-V Compound Semiconductors. Roman Talaksin1, Yuli Sigalovski2, Alex Galayuk1 and Yuri Makarov1, 2; STIR, Inc., Richmond, Virginia; 2Soft-Impact, Ltd., St. Petersburg, Russian Federation.

Introduction of simulation and modeling into development of MOVPE technology becomes more and more important in the last years [1, 2]. Modeling of MOVPE growth by both-gas and GaAs growth purposes. Besides the description of transport phenomena (flow, heat, species), an adequate chemistry model is necessary to predict deposition rates and uniformities and layer compositions. In this paper we present an integrated approach to simulation of III-V materials growth by MOVPE. The low temperature kinetic effects are described using a general mechanism - the blocking of group III species adsorption sites by methyl radicals. Deposition at intermediate temperatures that occurs under mass-transport limited growth conditions necessitates detailed modeling of transport processes accounting for reactor geometry features. These conditions are characteristic for MOVPE of group III arsenides and phosphides and the modeling results for this material will be presented. Another advantage of the formulated model is its ability to predict the growth rate and composition of the epitaxial layers at high deposition temperatures where the description of species from the surface is the rate limiting process. High temperature conditions are usually applied in MOVPE of group III nitrides and examples of the predictive modeling of the deposition of these materials will be given. The developed models have formed a basis for the development of an advanced simulator for MOVPE process. Materials systems considered in the tool are as follows: 1) epi-layers in the AlGaAs-GaAs system used for growing heterostructures for light emitting diodes, solar cells, laser diodes, high-electron mobility transistors, heterojunction transistors and vertical cavity surface emitting lasers. 2) epi-layers in the AlGaAs-GaAs system used for growing heterostructures for high-electron mobility transistors, light emitting diodes and laser diodes. The developed software is largely oriented to MOVPE engineers and researchers working both in industries and academia and is aimed to make modeling the routine and necessary step in new equipment and material design. [1] S.W. Benz, J. Mater. Sci. Mater. El. 13, 679 (2002) [2] S.Yu. Karpov, J. Crystal Growth 248, 1 (2003)

SESSION KK3: Poster Session I
Monday Evening, December 1, 2003
8:00 PM
Exhibition Hall D (Hynes)

KK3.1
Investigation of the Detailed Structure of Atomically Sharp Ge/SiO2 Interfaces. Tao Liu1, Wolfgang Windl1, Sergei Lopatin2,3, and Gerd Buchover4; 1Materials Science and Engineering, The Ohio State University, Columbus, Ohio; 2Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina; 3CMS Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Although the literature provides a multitude of (theoretical) structural models for Si/SiO2 interfaces, no method for experimental detection of the exact interfacial structure exists to date. In this paper we present a method for the refinement of the interfacial structure by a combination of theory and experiment, which we call AIDA-TEM (Ab-initio Doping Analysis by Transmission Electron Microscopy). The experimental part of AIDA-TEM consists of two TEM-based methods, Z-contrast imaging to study the segregation of heavy atoms and EELS for light elements, both with single-atom resolution. Z-contrast can detect the segregation sites of impurities with single-atom sensitivity even in amorphous as well as crystalline materials. EELS can detect the conduction band density of states (DOS) of the different atoms, which depends on the species as well as on the neighboring atoms. The same dopants are tested in theoretical calculations for their preferred segregation sites and conduction band DOS. The identification of key features of the winning structural models (whose dopant segregation and conduction band DOS patterns match the TEM findings) enables us then to propose reliable models for interface structures. In this paper we will apply AIDA-TEM to study the segregation behavior of Ge in oxidized Ge-implanted Si. Our results are commensurate with an atomically sharp interface.

KK3.2
New bond-order potentials for compound systems. Karsten Albe1, Paul Erhart1, Rune Nord2, and Kai Nordlund2; 1Institute of Materials Science, Materials Modeling Division, TU Darmstadt, Darmstadt, Germany; 2Accelemer Laboratory, University of Helsinki, Helsinki, Finland.

Atomic modeling of materials properties and processes on realistic time and length scales is mostly only possible if analytical potentials are used that are able to describe a variety of different material configurations. As it comes to technologically important systems realistic potentials are very often not available. Here we will report on bond-order potentials of the Brenner-Tersoff type that were recently developed for metal carbides, GdN, GdAs and SiC. We show that this angular dependent many-body potential type is not only capable to describe covalently bonded systems, but also to transition metals including heavy Rare Earth metals. The basic methodology and fitting scheme is presented and applications as well as shortcomings will be discussed by comparing with alternative schemes.

KK3.3
DFT Atomic-Scale Modeling of Mixed Co-Rh Transition-Metal Clusters. Samuel Demleitner1, Joseph Morillo1 and Gustavo M. Pastor1; 1CEMES, CNRS, CNRS, TOULOUSE, France; 2LPS/HEC, CNRS, TOULOUSE, France.

In the last decades, theoretical and experimental studies have demonstrated that size and dimensionality reduction of materials give rise to a large range of original physical and chemical behaviors [1]. This has opened the possibility of generating specifically designed nanomaterials with tailored properties. In particular, small transition-metal clusters are today the subject of considerable interest due to their possible applications in magnetic memories, catalysis and magnetic recording technologies. Alloying 3d and 4f elements is an effective way to combine a large magnetic moment with a high spin-orbit coupling due to the 4f strong spin-orbit coupling and the 3d high magnetic moments. Indeed, a strong enhancement of the magnetization in Co-Rh nanoparticles [2] compared to the bulk alloy value [3] was recently demonstrated. This motivates a systematic understanding of their magnetic properties, for which atomistic calculations are very fruitful. To this purpose small free Co12Rh13 clusters (N = 14513) have been studied [4] within the density-functional theory. In all cases the cluster geometry has been fully optimized from different initial configurations and for several relevant magnetic moments in order to locate the ground-state among the multiple closelylying isomers. The correlation between structural, chemical order and magnetic properties is analyzed. Comparison of magnetic and non-magnetic calculations reveals the significant role of magnetism on stability and cohesion. It appears that in most cases the average magnetic moment per atom is more than twice larger than in macroscopic alloys and increases with increasing Co concentration. The presence of Co induces a remarkable extension of the Rh local magnetic moments, in qualitative agreement with the experiment, while Co seems to retain its magnetic properties even in a highly mixed environment. For the larger icosahedral nanoparticles, in all cases there is a tendency to 4f surface segregation, associated to chemical disorder around the equicomposition. [1] P. Villieras-Gonzalez et al, Phys. Rev. B 55, 15684 (1997); [2] A.J. Cox et al, Phys. Rev. Lett. 70, 3323 (1993). [3] R.C. Proven et al, J. Magn. Mag. Mat. 243-246, 610 (2002); D. Zhang et al, Phys. Rev. Lett. 92, 247201 (2004); [4] S. Demleitner et al, J. Magn. Mag. Mat. 243-246, 610 (2002); S. Demleitner et al, to be published. [5] S. Demleitner, J. Morillo and G.M. Pastor, Surf. Sci. 537, 2-53.3, 334 (2003); Eur. J. Phys. D (in press, 2003).

KK3.4
Abstract Withdrawn

KK3.5

Cubic boron nitride has a wide field of applications due to its extraordinary physical and chemical properties. When using vapour deposition techniques such as ALD, the grown films usually become a mixture of various phases like c-BN, hexagonal BN and amorphous BN. To be able to optimise the growth of c-BN using thin film layer techniques, it is of highest importance to achieve a better understanding of the different reaction mechanisms that are occurring at the surface during the deposition. Therefore, various adsorption processes involving a (110)crystal surface of cubic BN has been investigated theoretically using a DFT approach. A three-dimensional alkyl model was used to simulate the surface. The various parameters that were used in the calculations of the adsorption energies have been chosen by performing a series of extensive test calculations, in which the effect of the parameters on adsorption energies has been carefully estimated. In order to prevent a collapse of the upper surface atoms (from a cubic to a hexagonal structure)
surface terminating species have to be induced in the model. This work focuses on H as a most promising saturating species. Its adsorption energy and geometrical structures have been calculated to both a surface boron and nitrogen atom. Furthermore, adsorption processes of several possible gaseous boron- and nitrogen-containing growth species have also been studied. The results show that NH and N$_2$ are too stable to become bonded to B, without any mixing of boron species. To nitrogen sites it is the boron species BH$_3$, BH$_4^-$ and BH$_2$ that are most suitable for growth on a (110) surface.

**K93.6**

Diamond growth in hydrogen-poor argon plasmas results in a polycrystalline film with grain sizes in the range of 3 to 10 nm. Growth mechanisms in this material have to be very different from conventional CVD growth. Unlike use of methyl radical and acetylene precursors in conventional diamond growth mechanisms, ultrananocrystalline diamond growth processes involve the C$_2$ dimer as predominant growth species. On the basis of calculated reaction mechanisms of C$_2$ with diamond surfaces, we are proposing a model that can account for very high remelting rates necessary to produce diamond with grain sizes in the nanometer scale. This nonempirical model invokes transition state theory to calculate reaction rates from the energies and barriers calculated using electronic structure methods. Resulting remelting rates and grain sizes provide a mechanism for nanocrystalline diamond growth in the absence of hydrogen. The dependence of remelting rate on a function of the C$_2$ density in the plasma was obtained from the model. It shows that a grain size reaches its maximal value at the temperatures of about 800°C. A comparison of the computed results with available experimental data is provided and further predictions are discussed.

**K93.7**

The Virtual Crystal Approximation has been used to study the structural and electronic properties of Nb$_{1-x}$Mo$_x$, Mg$_{1-x}$Al$_x$B$_2$, and MgB$_{1-x}$C$_x$. We show that the ab-initio VCA is useful in the study of metallic systems where the alloying elements are adjacent in the periodic table. The results were obtained by means of total-energy calculations using the full-potential Linearized Augmented Plane Wave method and the Generalized Gradient Approximation for the exchange-correlation potential. We present results for the structural parameters, elastic constants, and electronic structure. We find that the behavior of the calculated alloy band parameters differs from the Vegard's rule, in agreement with the experimental data. We show that the observed anomaly in the elastic constants of Nb$_{1-x}$Mo$_x$ around x=0.4 is an electronic topological transition effect. In addition, in the case of the lattice parameters of Mo$_{1-x}$Al$_x$B$_2$, and MgB$_{1-x}$C$_x$, we show that the experimental data of a(x) and c(x) for these alloys are reproduced by the calculations and the behavior is explained in terms of changes in the chemical bond. This research was supported by Consejo Nacional de Ciencia y Tecnología (CONACyT, Mexico).

**K93.8**
Crossover from tunnelling to the bulk scaling limit in correlated nanostructures. Jim Freericks. Physics, Georgetown University, Washington, District of Columbia.

We employ an inhomogeneous form of the dynamical mean field theory to examine transport in a device constructed of two ballistic metal leads and a barrier region. The barrier can be tuned through a metal insulator transition and its thickness can be varied from a single plane to temperature dependent junctions. The junction resistance as a function of the barrier thickness, the strength of the correlations, and the temperature. We see a crossover from an exponential dependence of the resistance on the barrier thickness to a linear dependence (indicating the bulk scaling limit has been reached). We extract appropriate energy and length scales that describe how this crossover occurs as a function of temperature. This analysis is useful to determine the parameter regimes where devices are dominated by quantum tunnelling effects.

**K93.9**
Modelling of W, Ti and Ta ALD precursors to determine penetration threshold in porous low k dielectrics. Thomas Abell$^1$, Ken Somers$^2$, Marc Hendrickx$^2$, Luc Vanquickenborne$^3$, Arnout Ceulemans$^2$ and Karen Maes$^3$; 1 Intel, Leuven, Belgium; 2 Dept. of Chemistry, K.U. Leuven, Belgium; 3 IMEC, Leuven, Belgium.

Atomic layer deposition (ALD) is an attractive method to deposit Cu diffusion barrier films for semiconductor interconnect applications due to the high conformational tendencies of ALD precursors. However, integration of ALD with porous low k dielectric materials is problematic due to the ability of gaseous ALD precursors to penetrate and deposit inside the porous structure of dielectrics that degrade their electrical properties. We attempted to estimate the penetration threshold of various precursor and probe molecules using Gaussian 98 modeling and a simple surface penetration schematic. The size and shape of precursor molecules for the deposition of Ti and Ta-based diffusion barrier materials (WNC, TiN, TaN, etc.) were modeled and fit to various geometric envelopes to determine the smallest pore diameter that these molecules could enter in their minimum conformations or configurations. For the WNC process, W$_6$F$_{18}$ was estimated to enter pores with a circular cross-sectional diameter of 12.3 Å. This indicates that the W$_6$F$_{18}$ will enter any material that will also allow penetration of the 8.6 Å diameter molecule toluene, the probe molecule for ellipsometric porosimetry. Deposition of W inside blanket films of microporous (<2 µm diam.) dielectrics was confirmed by XRR measurement and is documented for mesoporous (2 µm diam.) dielectrics. Triethylborane (TEB), one of the reactants in the WNC process, was estimated only to penetrate into circular cross-sections of 7.8 Å or elliptical cross-sections of 5.8 x 8.0 Å. This indicates the possibility of W$_6$F$_{18}$ penetration beyond TEB, a F getter, but not beyond the 3.8 Å NH$_3$ reactant. F etching at the interface of the deposition has been observed. Modeling of other molecular precursors for depth limiting is not possible. Due to the porous nature of barrier films, deposition processes such as PECVD and PDEAT were modeled for ALD TiN deposition indicating minimum elliptical cross-sections of 9.1 x 9.9 Å and 10.7 x 13.2 Å, respectively, for penetration. Calculations for precursors PECVD and PDEAT indicated ALD deposition of TaN films indicated elliptical cross-sections of 9.1 x 9.9 Å and 11.4 x 11.6 Å, respectively, for penetration. The Ti and Ta precursors are larger in cross-section which implies that they are less likely to penetrate into microporous dielectric films. It is also expected that the increased geometrical complexity of the molecules will hinder their movement inside the pore structure of a porous dielectric.

**K93.10**
Correlation of Atomic-scale Simulation to Experimental Results of the Formation and Growth of Oxide Nanostructures on Copper Thin Films. Richard John McAfee, Xuetian Han, Judith Yang and Guowen Zhou; Materials Science and Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania.

Parallel and personal computing systems can inexpensively perform simulations containing thousands of atoms, whereas experimental methodologies are approaching the same spatial and temporal scale as simulations under highly controlled conditions. The work presented here produces current flow and barrier parameters from the Kinetic Monte Carlo (KMC) and Molecular Dynamic (MD) computer simulation of island nucleation and growth of CuO islands to directly correlate with in situ Ultra High Vacuum Transmission Electron Microscopy (UHV-TEM) experiment. Simulations of copper thin films oxidized at various temperatures and pressures of oxygen. Copper passivation is critical to understand at the nanoscale since a recent advance in microprocessor design allowing for increased speed and reduced operating temperatures for the replacement of gold interconnects with copper as the interconnect material. The effect of oxidation on the properties and performance of the interconnect material becomes more significant as the dimensions decrease. Additionally, the spatial distribution of oxide islands on a metal substrate may form in a selforganizing manner, important in nanotechnology applications. In-situ oxidation experiments of Cu(100) at low pressures of oxygen at 600°C show similar island morphology to Ge grown on a Si substrate. Therefore, the theory and body of work available for semiconductor simulation provides a starting point and the algorithms. Initial simulation results show reasonable agreement with experiment. The effect of various simulation parameters on results may allow for better understanding of the materials science of nanoscale oxidation and new improved manufacturing techniques to prevent problems resulting from oxidation, to add new functionality, and to reduce cost. Methods developed for this system will be applicable to systems other than metal-oxides.

**K93.11**
Ab initio based modeling of transition metal monoxides having defect lattices. D. A. Anderson$^1$, P. A. Korzhnev$^1$ and B. Johnson$^1$$^2$; 1 Materials Science and Engineering, Royal Institute of Technology, Stockholm, Sweden; Physics, Uppsala University, Uppsala, Sweden.

The presence of defects (vacancies, interstitials, etc.) in materials...
based on transition metal oxides influence their chemical and physical properties, such as stability, catalytic activity, diffusivity, hardness and electrical conductivity. Experimental measurements of these defects and interpretation of the results are often difficult due to the complexity of these materials. Theoretical calculations based on quantum mechanics can nowadays be a complementary way of obtaining information about defects and their behavior in oxide materials. In the present paper this will be exemplified by results for titanium and vanadium monoxides. Transition metals in groups IV and V in the periodic table tend to form oxides based on the cubic NaCl structure with stoichiometric composition. Titanium and vanadium monoxides can have large fractions of vacancies on both the metal and non-metal sublattices. Depending on the temperature and pressure these vacancies can either be ordered or disordered. We have treated the ordered structures with a pseudo-potential method using a plane wave basis set, while the calculations for the structures with disordered vacancies were performed within the framework of the muffin-tin orbital Green’s function technique. For TiO our calculations confirm that a monoclinic vacancy-containing phase is stable at low temperature and pressure. At high pressure a transition to the vacancy free NaCl structure is predicted. The transition from the structure with disordered vacancies to the NaCl structure has experimentally been shown to occur at much lower pressures and it is discussed how this relates to the present theoretical results for defect containing and defect free TiO. The stability, conductivity as well as the structural and mechanical properties of TiO and VO are discussed in terms of the electronic structure. The authors gratefully acknowledge support from the Swedish Foundation for Strategic Research through the Center for Computational Thermodynamics (CCT).

K3.12
Abstract Withdrawn

K3.13

In recent years, new formulations of the virtual crystal approximation (VCA) have been devised. These implementations have improved upon previous versions of the VCA, which provided in some cases only qualitative agreement with experimental and large-scale solid-state calculations. One new method focused on constructing a VCA potential that possesses correctly averaged electronic atomic properties [Phys. Rev. B 62, R245 (2000)]. This method, however, was formulated for averaging homovalent atoms into the virtual atom. In the case of heterovalent atoms, this method can be reformulated using non-trivial averaging methods for the atomic potentials and atomic orbital energies. This heterovalent VCA formulation has been utilized to study Mg1/2Al1/2. Electronic properties for the VCA atom are compared to all-electron results for the component atoms.

K3.14
The Constant Traction Method For Molecular Dynamics Simulations of Systems Under Mechanical Loading. Polonizio Ciavatta, Luciano Colombo,1, Unità Materiali e Nanoscienze, ENEA CNR, Cisano San Pietro, Italy,1 INFM and Dipartimento di Fisica, Università Cattolica, Rome, Italy.

We describe the constant-traction molecular dynamics method to perform simulations on generic atomic systems under an applied external load at finite temperature. The main object of the method is to ensure consistency between the atomistic model and the macroscopic continuum mechanics description (the Cauchy-Binder principle). Examples of simulations for different kinds of extended defects under an external load, such as a grain boundary, an elliptical microrcrack and a screw dislocation in an fcc crystal are presented, and compared with the results of the corresponding continuum mechanics description. Recent developments in the extension of the method to semi-empirical and ab-initio molecular dynamics will be discussed.

K3.15
Ab initio study of dislocation clusters in silicon. Dmitry Mishin and Laurent J. Lewis, Department of Physics, University of Montreal, Montreal, Quebec, Canada.

At room temperature, vacancies resulting from irradiation of silicon are mobile and quickly form dislocations. The presence of dislocations can be detected using, in particular, infrared or positron annihilation spectroscopy. However, for vacancy annealing at T=550 C, there is a contradiction between the results given by these two methods: whereas infrared absorption decreases quickly with time, the positron lifetime remains unchanged [1]. In order to understand this phenomenon, we first simulated the formation and positron lifetime for dislocation clusters in various configurations. The calculations were performed within the pseudopotential DFT method. Positron lifetimes were computed using unperturbed electron densities taken from DFT calculations, while the core potential was the simple trivalent or annihilation enhancement factors were determined within the semiconductor model [2]. It is found that there exists configurations consisting of nearly (but not directly bound) dislocations that have quasi low formation energy. It is proposed that the interaction between the dislocations may change the optical properties of the system, while leaving the positron lifetimes unchanged. [1] R. Poirier et al, Nucl. Instr. Meth. in Phys. Rev. B, 206 (2000) 85. [2] M.J. Puska et al, Phys. Rev. B, 30 (1984) 7699.

K3.16
Theoretical Study of Point Defects in ZrO2-Silicon Interfaces. Masashi Nakatomi and Koichi Yamauchi, University of Tokyo, Tokyo, Japan.

We present a numerical study of point defects in ZrO2-silicon interfaces. The structure of ZrO2-silicon interface has been determined by molecular dynamics calculations. We used a slab model that consists of nine atomic layers of silicon and nine atomic layers of ZrO2. Three atomic layers of the slab that containing seventeen oxygen atoms, eight silicon atoms and nine Zr atoms correspond to a ZrO2-silicon interface. We then have performed density functional theory calculations to investigate the band structure of the interface using the plane wave basis VASP code. The results demonstrate that lengthen Zr-O bonds and interstitial oxygen atoms give defect levels in the band gap. In particular, the defect levels due to interstitial oxygen atoms are locate closely on the top of the valence band, and may therefore affect the efficiency of gate dielectrics.

K3.17
Molecular Dynamics Simulation on the Morphological Transformation of Dislocation Loops in FCC Metals. Hideo Kurokuki1, Tomoko Kudoyoshi1, Futoshi Shimizu1, Hajime Kimizuka2, Shiro Jitsukawa3 and Ju Li4, 1Center for Promotion of Computational Science and Engineering, Japan Atomic Energy Research Institute, Tokai, Horiaki, Japan; 2Energy and Environment Technology Department, The Japan Research Institute, Tokyo, Japan; 3Department of Materials Science, Japan Atomic Energy Research Institute, Tokai, Japan; 4Department of Materials Science, The Ohio State University, Columbus, Ohio.

Irradiation of FCC metals by charged or neutron particles induce atomic collision cascades, where vacancies and interstitials aggregate to form varieties of clusters ranging from nano- to micrometer-size. Typical clusters in FCC metals, which are observed in the transmission electron microscope and influence significantly the mechanical properties of irradiated materials, are hexagonal interstitial and vacancy dislocation loops with stacking fault inside. Also, stacking fault tetrahedra and unfaulting of dislocation loops are frequently observed, however their formation process and transformation mechanism have not been known in detail. We performed large-scale molecular dynamics simulation using the EAM potential of Cu and Al combined with the visualization techniques for defects to study the dislocation process of dislocation loops, and, in particular, successfully observed that fully dissociated dislocation loops of various sizes transform to other structures under specific conditions. From these results, we have found the critical condition for the self-organized formation of a stacking fault tetrahedron from the dissociation of modified hexagonal vacancy dislocation loop. With this visualization of the transformation of the dislocation loops, we have also found atomistically the unfaulting process of a dislocation loop where Shockley partials are emitted to the stacking fault leading to a perfect dislocation loop. We also present the atomistic result on the interaction of an edge dislocation with the above clusters and the relation to the mechanical properties of materials.

K3.18
Dislocations and Grain Boundaries in Polycrystalline Tungsten Wires. Matias Mrovec1,2, Christian Elmerser3, Peter Gumbsch1,2 and Vadke Virk3, 1Fraunhofer IWM, Freiburg, Germany, 2HZS, University of Karlsruhe, Karlsruhe, Germany, 3University of Pennsylvania, Philadelphia, Pennsylvania.

The mechanical properties of polycrystalline tungsten wires are controlled by the motion of screw dislocations and their interaction with grain boundaries. In our study we have investigated the structure and energetics of these extended defects using bond-order potentials that are based on tight-binding theory. The validity and transferability of the potentials have been verified by comparison to the results of first principles calculations for several simple structures including the [211] twin boundary and its shear resistance. Large scale calculations of several other grain boundaries and of the interaction of a dislocation with these boundaries are then performed using the bond-order potentials.
Surface Segregation Energies of BCC Binaries from Ab Initio and Quantum Approximate Calculations. Brian S. Good, NASA Glenn Research Center, Cleveland, Ohio.

We compare dilute-limit segregation energies for selected BCC transition metal binaries computed using ab initio and quantum approximate energy methods. Ab initio calculations are carried out using the CASTEP plane-wave pseudopotential computer code, while quantum approximate results are computed using the Holzboog-Sieger-Smith (HFS) method with the most recent parameterization. Quantum approximate segregation energies are computed with and without atomic relaxation. The ab initio calculations are performed without relaxation for the most part, but predicted relaxations from quantum approximate calculations are used in selected cases to compute approximate relaxed ab initio segregation energies. Results are discussed within the context of segregation models driven by strain and bond-breaking effects. We compare our results with earlier approximate and ab initio theoretical work, and available experimental results.

Direct Experimental and Simulation Comparisons of the Nanoscale Oxidation Behavior of Cu(100). Xuefan Han, Rich McAfee and Judith C Yang; Materials Science and Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania.

Surface oxidation process plays critical roles in environment stability, high temperature corrosion, electrochemistry, catalysis and some thin film growth. Because of its importance, much work has been done to investigate this process using many different techniques, yet fundamental understanding of the initial oxidation kinetics, from the oxide nucleation to coalescence, is still surprisingly not well understood. We have extensive experimental results of the nanoscale oxidation process of Cu(100) thin films in situ UHV-TEM at various temperatures and oxidation pressures. The initial oxidation kinetics shows a striking resemblance to heteroepitaxy, where oxygen surface diffusion is the primary mechanism of CuO island nucleation and growth. Yet, theoretical analysis is necessary for deeper understanding of these nanoscale processes. In this paper, a simulation program based on the kinetic Monte Carlo method, to directly correlate with the experimental observations, will be introduced. By using this program, the two dimensional Cu(100) oxidation behavior can be simulated with various initial and final conditions. Some correlations, like deposition rate vs. nucleation rate, temperature vs. saturated island density and temperature vs. sticking probability, are being established. A reasonable match of the simulated data and the experimental data has been found. This simulation effort effectively evaluates the in situ experimental results and it is essential for the fundamental understanding of the nanoscale metal oxidation reactions.

A Nonorthogonal Tight Binding Hamiltonian for the Study of Nanocrystalline Materials. Anna Maria Musumeci, Istituto IMM, CNR, Bologna, Italy.

Many current researches in solid state physics and in material science focus on nanocrystalline materials. These materials are formed by the assembly of crystalline grains with nanometer dimensions and their features may noticeably deviate from the ones of the parent solid. In spite of extensive efforts concentrated in this field, the understanding of these effects is generally qualitative and is jeopardized by the large structural size of the grains which is beyond the present capabilities of ab initio models. With the aim of a computationally efficient and physically accurate method in this study we present a nonorthogonal tight-binding Hamiltonian based on the extended Hückel approximation. A versatile parameterization, which elaborates on current models, has been developed to describe large structures of compound composition and with a complex shape. The Hamiltonian has been extensively tested on a wide range of structures, i.e., bulk materials, surfaces and small clusters of either metallic and covalent composition. In the field of nanocrystals the method has been applied to tin dioxided crystalline grains, a material of both theoretical and practical relevance due to its use for solar cells, heat reflecting filters and as a gas sensor.

Molecular Dynamics Simulation of Stress and Capillarity Induced Grain Boundary Migration in Nickel. Hao Zhang, Mikhail I Mendeleev7, and David J Skrokiv7; Princeton Materials Institute, Department of Mechanical and Aerospace Engineering, Princeton Materials Institute, Princeton, New Jersey.

Control of crystallographic texture during materials processing is key to achieving a wide range of desirable physical properties. All processes that modify texture are based upon microstructural evolution occurring through the motion of grain boundaries. Quantum mechanical simulations of microstructure evolution must be based upon grain boundary mobilities, which are functions of the five crystallographic parameters that describe each grain boundary. We will present the results of a series of studies of 3-d molecular dynamics simulations of grain boundary migration as a function of grain misorientation and grain boundary inclination. These studies were performed with embedded atom method type potentials fitted to represent nickel. In the first study, stored elastic energy was used to drive migrating grain boundaries. In the second study, the grain boundary mobility was found to be linear function of driving force for all grain boundary misorientations and inclinations. Simulations performed at different temperatures were used to calculate the activation energy for boundary migration. In the second study, we simulated steady-state curved driven boundary migration in a half-circle geometry for the same boundary misorientations used in the first study. These simulations provide a means of determining reduced approximations and input parameters (the product of the grain boundary mobility and stiffness). Together, these two data sets allow us to answer the outstanding question “does grain boundary mobility depend on the nature of the driving force?”

SESSION KK4: Nano-systems, Surfaces, and Interfaces
Chair: Anneli Korin
Tuesday Morning, December 2
Constitution A (Sheraton)

8:30 AM KK4.1 Carbon Nanotubes Structures and MD Simulations at the Realistic Limit. Kimmo Kaski, Maarit Hakulinen and Antti Karonen, Research Centre for Computational Science and Engineering, Helsinki University of Technology, ESPOO, Finland.

Carbon nanotubes as all-carbon molecules of tubular form exemplify modern nanometer scale material structures, where the number of atoms ranges from less than a million up to tens of millions. Such systems are quite ideal for the study of simple molecular dynamics (MD) simulations because they can be done at the realistic limit, rendering them in a way predictive. However, the goodnes of their predicative is dependent on the model potential, for which the empirical potentials developed by Brenner have turned out to be quite successful, e.g. in describing structural properties of single walled tubes (SWT’s). Nevertheless, in cases like the SWT under strong bending where structural deformation can be large and defects form, more accurate dynamical tight-binding method needs to be used in conjunction. Since the TB method is limited for studying systems of the order of thousand atoms we have focused it only to areas of large deformations in the tube. In this report we demonstrate that the joint use of MD and dynamical TB simulations can yield insight to carbon nanotube structures and their deformations.

9:00 AM KK4.2 Ballistic Conductance of Functionalized Carbon Nanotubes: First-principles Simulation. Young-Soo Lee, Marco Buongiorno Nardelli and Nicola Malossi; 1Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; 2Department of Physics, North Carolina State University, Raleigh, North Carolina.

Functionalization of carbon nanotubes has drawn much attention due to their potential applications e.g. as bio/chemical sensors or in electronic devices. In the interest of controlling electronic properties, sidewall functionalization represents a very promising avenue since the delocalized pi bonding is vulnerable to covalently attached functional groups. High degree of sidewall functionalization has been reported; however, in collapse of such the change distribution is dictated by functional groups and whether it preserves other unique and versatile properties of the clean carbon nanotubes. In this work, we calculate the ballistic conductance of functionalized nanotubes using first-principles simulations of C60-Parrinello molecular dynamics with the maximally-localized Wannier-function method allows us to deal with relatively big systems and to investigate the bonding in the chemically-modified region. We focus here on the variation of conductance obtained by attaching electron-donating and electron-accepting functional groups.

9:15 AM KK4.3 Development, validation, and application of mesoscopic theory and simulation for quantum dot formation. Abhijit Chatterjee, Dimitrios G. Vlahos and Konstantis A. Markou; 1Department of Chemical Engineering and Center for
Formation of periodic domains of nanoparticles on growing films, such as semiconductor quantum dots, metallic nanoparticles and nanowires, via self-organization routes occurring through cooperative phenomena where intermolecular forces and strain-induced interactions are critical. Molecular simulation tools, such as kinetic Monte Carlo (KMC) algorithms use a molecular level description of the intermolecular potential interactions, and therefore, are dealt tools for studying pattern formation of nanoparticles on surfaces. However, KMC simulations are limited to short length and time scales, whereas experimental data often involve scales beyond the realm of these atomistic simulation tools. This is particularly the case for long-range strain-induced interactions. In this talk, we introduce novel coarse-grained Monte Carlo (CGMC) simulations that can be used to link the microscopic scales with self-organization phenomena in the scale of nanometers. We also show how the competition between coarsening and demixing in a system allows to estimate coarsening rates, which are relevant for understanding the interplay of both phenomena. This can be achieved by identifying conditions where nanoparticle self-organization occurs.

9:30 AM KK4.4 Laser-Focused Atom Deposition on Anisotropic Substrates,
2D Monte Carlo Simulation: Florin Nita and Alberto Pimpinelli
LASMEA, Blaise Pascal University, Clermont-Ferrand, France; Institute of Physical Chemistry, Romanian Academy, Bucharest, Romania.

Last year a lot of efforts were made, in the beginning to obtain, and after that to improve the quality and the density of the nanocluster arrays. One of the techniques used to obtain such arrays is the Laser-focused atom deposition. A standing wave region is created in the proximity of a crystal surface, if a laser beam is directed parallel to this surface and then retracted. The wavelength of the standing wave is 1/2 where λ is the optical wavelength, and this region acts like an array of cylindrical lenses for an incoming neutral atoms beam. The role of the surface diffusion anisotropy in the fabrication of nanostructures by laser-focused ("cold") ion lithography, and on the stability of these nanostructures is studied using 2D kinetic Monte Carlo simulations. Two different wave profiles were used in the simulations. The simulations were performed using one- and two-dimensional standing wave fields and two different diffusion models (limited and total diffusion model) on nanotribes, such as (110) surfaces of FCC crystals, or reconstructed surfaces such as Si(100). The simulations were made with and without Schwoebel barriers. Our diffusion-deposition models reproduce both qualitative and quantitative experimental results. They show that the time evolution of height, FWHM and background for the profiles obtained using the same standing wave are different for different orientations of the standing wave fields, and that the change of the direction of the incident on the surface: parallel (∥) and perpendicular (⊥), respectively. Our results suggest that it is possible to reduce the feature width in nanostructures, such as quantum dots or quantum wires, using laser-focused ion deposition techniques on an anisotropic substrate. This work was supported by EC Contract No. IST-2001.32264 (NANOCLD).

10:15 AM *KK4.5 Variable Stoichiometry, Defects and Reactions at Oxide Surfaces, Nicholas Harrison, Chemistry, Imperial College London, London, London, United Kingdom.

Under the operating conditions of many devices oxide surfaces are highly defective, often reconstructed and may have a stoichiometry different from that of the bulk crystal. The electronic and magnetic structure of the surface may be very different from that of the bulk or idealised surfaces. In many applications, particularly those which depend on nanostructured materials, materials design depends on the control of the surface electronic and magnetic properties. Recent developments in first principles simulation have significantly increased the reliability of the computed ground state energy surfaces in strongly interacting oxides. It is now not unrealistic to attempt to predict the stoichiometry, electronic and magnetic properties for rather complex systems under realistic operating conditions. These developments will be reviewed and their application to the surface electronic structure and magnetism in a number of transition metal oxides will be discussed.

10:45 AM KK4.6 Ab-initio Simulations of Homoepitaxial Growth of SiC(111), Maria Chinna Righ1,2,3,4, Carlo Antonio Pignedoli1,2,3,4, Alessandra Costamagna2,3,4, Renato Del Felice1,2,3,4 and Carlo Maria Bertoni1,2,3,4
INFN-National Research Center on Nanomaterials and BioSystems at Surfaces (SR), Modena, Italy; 1Dipartimento di Fisica, Università di Modena e Reggio Emilia, Modena, Italy; 2CNR-IMM, Pisa, Italy.

Silicon Carbide (SiC) is one of the most promising wide-bandgap semiconductors for harsh environment applications. The development of SiC-based technology was so far delayed because of difficulties in the material production. Experiments of solid-source molecular beam epitaxy have shown that an accurate SiC layer-by-layer growth on SiC(111) surface is possible under stabilized conditions [1], suggesting that the surface reconstruction plays a relevant role in determining the growth mode and the film quality. We investigated this point by simulating the initial stages of β-SiC growth on the SiC(111)-α srp3 x α srp3 surface. We found that the surface reconstruction influences the kinetics of adatom incorporation in such a way that a layer-by-layer growth may be favored: the local environment of the α srp3 x α srp3 reconstruction shapes a multilevel potential energy surface for the deposited C atoms that induces their channeling towards the correct crystalline sites. Moreover, the anisotropic substrate C diffusion, along with the observed C-C interactions, favors the nucleation around each Si adatom of the original reconstruction. The formation of several small islands, instead of large islands in conducive to a layer-by-layer growth. In addition to this, our quasistatic quantum mechanical simulations reveal that the gain in surface energy obtained by capping the growing surface with the right dose of Si atoms that are necessary to recover the α srp3 x α srp3 reconstruction, is sufficient to initiate the spontaneous transition of the system from a metastable defective configuration to the SiC crystal structure, thus revealing a surface-driven mechanism able to stabilize defect-free layer-on-layer deposition on high surfaces. [1] A. Pisani et al., J. Appl. Phys. Lett. 66, 3185 (1995); Appl. Phys. Lett. 68, 1204 (1996).

11:00 AM KK4.7 Elastic Interaction of Oxygen atoms on a Graphite basal Plane, Philippe Peylin, Andrei Incze and alain pastier, LMP2C, Universite Joseph Fourier, Grenoble, France.

We calculate the elastic interaction energy between two oxygen atoms deposited on a graphite basal plane. Simulations are performed with ab initio calculations (VASP) and continuum theory of elasticity. The comparison between the results obtained with the two different methods, despite their usual length scale domain of application, is very good, attractive and repulsive behaviors are found. We speculate that this type of interaction could play an important role in the rearrangement of oxygen atoms experimentally observed after a weak oxidation of a graphene surface. First results about elastic interaction of oxygen atoms on a graphite surface have been published in Phys. Rev. B66, [Brief Report], 172101 (2002).

11:15 AM KK4.8 Atomic and electronic structure modelling of nanoamorphous films in silicon nitride ceramics (4+), Duc Nguyen-Minh, David J.H. Cockayne1, Markus Doeblinger2, Adrian Sutton1 and Adria van Dun1,2, Department of Materials, University of Oxford, Oxford, United Kingdom; 1Bedeck Institute, California Institute of Technology, Pasadena, California.

The presence of the thin intergranular films (IGF) between crystals can significantly influence mechanical, thermodynamic and chemical properties of bulk ceramic materials. Because of this, there is increasing interest in understanding the local bonding structures of the IGF and a variety of modelling and experimental studies are being used to investigate the IGF structures. The chemical, structural, electronic, and mechanical properties of the IGFs depend on the IGF thickness and the chemistry of the adjacent grains. Molecular dynamic (MD) simulations have been performed to investigate the nanostructure of nanoamorphous IGFs formed between various basal and prism planes of silicon nitride crystals. We found that bonding formation of Si-N and Si-O bonds are dominant in stabilizing silicon oxynitride.
film, a formation of nitrogen triple-bond dimers is observed during the MD runs at 2000K. We have studied the dependence of ratio N/(N4) on a crucial role in the dynamical properties of Si-O-N amorphous films, on different temperature regimes and IGFs thickness. Our MD simulations show that the N2 formation is substantially reduced when the ratio N/(N4)=0.8 which is in good agreement with electron energy loss spectroscopy (EELS) quantitative studies of composition and chemical profiles in interfacial regions. The calculated radial distribution function decomposes into different contributions and compared with those experimentally measured using nanosecond x-ray diffraction techniques. Finally, the bond-order behaviour across the IGFs is analyzed in details from simulated interfacial atomic structures within both RRI framework and DFT electronic structure calculations from an all-atomic tight-binding PLATO code. (4) This work is supported by UC/US collaborative grant (GRD2-200-300T) on "Nanometer scale induced structure between amorphous layers and crystalline materials".

11:30 AM K4K.4 Hybrid Atomic/Continuum Model for Multi-Scale Simulation of Surface Evolution: Paul Spencer, Simon Gill and Alan Cooke, Department of Engineering, University of Leicester, Leicester, United Kingdom.

A combined atomic/continuum scale method to simulate the evolution of a surface via diffusion is presented. The atomic scale description uses the Kinetic Monte Carlo (KMC) method to simulate diffusion as discrete random hopping events. The continuum description represents diffusion as a deterministic flux. The Hybrid scheme links the two descriptions using a Blending Regime. Both atomic and continuum chemical species are simultaneously represented in the region allowing material to move across the KMC/continuum interface in a consistent manner. This method naturally allows for the co-existence of multiple length and time scales within a single simulation. The effectiveness of the scheme is demonstrated using a Solid-Solid potential for simple surface profiles.


The development of molecular scale electronic devices has been hampered by the experimental difficulties associated with contacting and measuring the electrical properties of individual molecules. It must be equally acknowledged that theoretical treatments of charge transport across molecular devices are hampering molecular electronic design efforts due to problems such as the large discrepancies found between calculated and experimental current-voltage characteristics, and as well disagreement between differing theoretical treatments. Typically, theoretical treatments predict currents two to three orders of magnitude higher than experiment. It is desirable to be able to apply the highly developed methods of quantum chemistry and electronic structure theory to the practical problem of designing atomic scale electronic devices and components. However, it remains a difficult problem to extend the machinery of electronic structure theory, largely developed to study closed or periodic systems, to incorporate open systems and boundary conditions needed to describe electronic transport. If open boundary conditions are introduced into density functional theory (DFT) calculations, several problems arise. For example, the exchange-correlation functional is current dependent, a fact not explored in detail within molecular electronic studies. Recently, it has been highlighted that the currents theoretically predicted with DFT methods can vary by over an order of magnitude simply due to the choice of exchange-correlation functional. A further problem is that application of a single particle distribution function to the Kohn-Sham eigenvalues is an ambiguous procedure. In our approach to the electronic transport problem, we side step these issues by minimizing the energy of a molecule in contact with metallic contacts, within-body basis and with open system boundary conditions formulated in a manner appropriate to the case of correlated many-body wave functions. Application of the method leads calculation of current-voltage characteristics for prototypical molecular systems within the same order of magnitude as experimental observations.

SESSION KK5: Methods I
Chair: Jim Greer
Tuesday Afternoon, December 2, 2003
Constitution A (Sheraton)

130 PM *KK5.1 Real-space Multiscale Simulations for Metals: Implementation of Density-functional with Embedded Atom Coupling: Efthimios Kaxiras1,2, Nick Choly1, Gang Li1 and E. Weinrib1 1Physics, Harvard University, Cambridge, Massachusetts; 2Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts.

The use of multiscale simulations for materials is evolving into a major theme in the treatment of realistic systems. Applications to covalently bonded systems have already been successfully performed, incorporating all the relevant length scales from the quantum mechanical to the continuum. What has made such seamlessly coupled schemes feasible is the possibility of embedding quantum mechanical calculations from an all-atomic tight-binding PLATO code. (4) This work is supported by UC/US collaborative grant (GRD2-200-300T) on "Nanometer scale induced structure between amorphous layers and crystalline materials".

2:00 PM KK5.2 Multiscale Modeling of Small Molecules in Zeolite-4A: N. A. Modine, M Chandross and E Jarmillo; Sandin National Labs, Alburquerque, New Mexico.

Confinement within the nanoscale pores of a zeolite strongly modifies the physical and chemical behavior of small molecules such as water, ammonia, and carbon dioxide. Realistic modeling of such phenomena requires simultaneously capturing the detailed behavior of chemical bonds and the possibility of collective dynamics occurring in a complex unit cell (672 atoms in the case of Zeolite-4A). Classical simulations alone cannot reliably model the breaking and formation of chemical bonds, while quantum methods alone are incapable of treating the extended length and time scales characteristic of complex dynamics. Therefore, we have taken a mixed quantum/classical approach. We report our progress in developing an efficient algorithm for embedding a small region of high density functional theory within a larger system represented by classical potentials. We compare Green's function and energy minimization approaches to finding a localized representation of the electronic structure, and we discuss results for the behavior of water, ammonia, and carbon dioxide in Zeolite-4A. Sandin is a multiprogram laboratory operated by Sandin Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85009.

2:15 PM KK5.3 From DFT to TB: The Mo-C system: Mitos Mross1,2, Rebecca Jansch1 and Christian Elsasser1; 1Forschungszentrum Juelich, Juelich, Germany; 2Max-Planck Institute of Metals Research, Stuttgart, Germany.

In the course of developing a multi-scale model for the description of chemical vapor deposition growth on metal films on metal substrates we have investigated the Mo-C system in a substrate film case study. In order to describe the system as various length and time scales, different methods are needed. As the initial step, the system has been investigated by means of the density functional theory with the mixed-basis pseudopotential approach. The results of these ab-initio calculations provide us with extensive information about global and local electronic properties of various phases in the system and serve also as a benchmark for less rigorous schemes. The database of first-principles results is used for the construction of two semi-empirical schemes: the environment-dependent tight-binding model (EDTB) of Hans et al and the bond-order potentials (BOP) of Porteau et al. These two models are based on the tight-binding theory but they differ in underlying mathematical formalism and physical applicability. While EDTB is a traditional k-space method, BOPs are cast in the real space. Here we present first results assessing the performance and reliability of both models for application in large scale simulations.
2:30 PM KK5.4
Development of New Tight-Binding Quantum Chemical Molecular Dynamics Method and Its Application to Electronic Materials. Momoji Kubo1, Natsuki Iido2, Takahiro Oyama3, Katsumi Sasa4, Akira Endo1, Akira Immura2 and Akira Miyamoto5,6, 1Department of Applied Chemistry, Graduate School of Engineering, Tohoku University, Sendai, Miyagi, Japan; 2Department of Mathematics, Faculty of Engineering, Hiroshima Kokusai Gakuen University, Hiroshima, Hiroshima, Japan; 3New Industry Creation Hatchery Center, Tohoku University, Sendai, Miyagi, Japan.
Recently, we succeeded in the development of new tight-binding quantum chemical molecular dynamics method, which realizes more than 5,000 times acceleration compared with the regular first-principles molecular dynamics method. It indicates that 10 years calculation by the first-principles molecular dynamics can be finished within only one day by our accelerated quantum chemical molecular dynamics method. Methodology enables to perform the large-scale simulations and to clarify the chemical reaction and electron transfer dynamics in the electronic materials. We successfully applied the above method to the etching process, chemical mechanical polishing process, crystal growth process, and various processes related to the electronics materials fabrication [13]. The chemical reaction dynamics and electron transfer dynamics during the above processes were clearly elucidated by using our new program. Especially, we succeeded in the first time to fabricate plasma display and the validity of our designed materials is experimentally investigated. Finally, we confirmed that our accelerated quantum chemical molecular dynamics program is a very powerful tool to solve a level dynamics and to design new electronics materials [1]. T. Yokosuka, H. Kurokawa, S. Tkami, M. Kubo, A. Miyamoto, and A. Immura, Jpn. J. Appl. Phys., 41 (2002) 2411. [2] K. Satara, T. Yokosuka, H. Kurokawa, S. Tkami, M. Kubo, A. Immura, K. Shimura, M. Kakeshita, and A. Miyamoto, Jpn. J. Appl. Phys., 42 (2003) 1859. [3] T. Yokosuka, K. Satara, H. Kurokawa, S. Tkami, M. Kubo, A. Immura, and A. Miyamoto, Jpn. J. Appl. Phys., 42 (2003) 1857.

3:15 PM *KK5.5
Transformation of Harrison’s Tight-Binding Theory from a Qualitative Approach to a Quantitative Tool. Lei Shi1 and Douglas A. Pincus2, 1Virginia Commonwealth University, Richmond, Virginia, 2Center for Computational Materials Science, Naval Research Laboratory, Washington, District of Columbia.
Harrison’s tight-binding theory (TB) [1] provides an excellent qualitative picture of electronic structure of the elements across the periodic table. However, Harrison’s universal TB parameters produce energy bands and densities of states that are in serious disagreement with the results one gets from standard density functional theory [2] or the APW, LMT0 or pseudopotential methods. In this work we have developed a procedure that maintains the simplicity of Harrison’s approach but gives an improved solution for the total energy, its derivatives, and a quantitative basis [3]. To accomplish this we proceed as follows: 1. We introduced the p-only energy as the only additional parameter to the s and d on-site energies used by Harrison, and increased the size of the secular equation to just p in the Hamiltonian. Our method simultaneously the APW energy bands of hcp Nb and fcc Pd using as adjustable parameters the above three on-site energies, Harrison’s parameter R0 and the ten prefactors of the two-center integrals, keeping Harrison’s functional form. 2. We kept the ten prefactors determined above as frozen, and then we fitted the all the 3d, 4d, and 5d elements using the on-site energies and R0 as adjustable parameters. We did the above fitting at the experimental value of the lattice constants and we reproduced the APW results remarkably well. With the inclusion of one additional parameter we also have been able to describe the lattice constant dependence of the energy bands. We believe that our scheme will work equally well for sp elements, will also describe total energies and has applications for and equations in binary materials [1]. W.A. Harrison, “Electronic Structure and the Properties of Solids,” Dover Publications, Inc., New York 1988. W.A. Harrison “Elementary Electronic Structure,” World Scientific 1999

3:45 PM KK5.6
Full-potential Locally Self-consistent Multiple Scattering (FP-LSMS) Method, Malcolm Stock1, Aurelian Rusnau2, Yang Wang3, Don Nicholson4 and J.S. Farkas5, Purdue University, West Lafayette, Indiana; 2Oak Ridge National Laboratory, Oak Ridge, Tennessee; 3Department of Physics, Florida Atlantic University, Boca Raton, Florida.
In this presentation, we introduce the Full-potential Locally Self-consistent multiple scattering (FP-LSMS) method that we recently developed. The FP-LSMS method is an order-N approach to the ab initio electronic structure calculations for solids. It is based on full-potential multiple scattering theory, and allows to eliminate the multipole approximation for both potentials and charge densities. In the parallel implementation of the method, we allow multiple atoms to be distributed on each processor. We also implemented the screened structure constants with sparse matrix algorithm which speeds up the multiple scattering matrix calculation significantly. We will demonstrate the order-N scaling of the method, and we will also show a preliminary application of the method.

4:00 PM KK5.7
First Principles Molecular Dynamics in a Uniform Magnetic Field. Wei Cai1 and Giulia Galli; Chemistry and Materials Science, Lawrence Livermore National Lab, Livermore, California.
While ab initio, plane-wave methods in the absence of external fields are widely used because of their computational efficiency, ab initio electronic structure calculations and first principles molecular dynamics simulations in a finite, uniform magnetic field have not yet been attempted. To treat a uniform magnetic field non-perturbatively, the Hamiltonian needs to depend on a vector potential that destroys translational invariance, thus making the use of plane-wave basis impractical. A new method is presented which allows one to perform ab initio calculations in a finite magnetic field by retaining the computational efficiency of plane-wave like basis and fast Fourier transform techniques. This method has been successfully applied to systems such as an interacting electron gas in quantum wells and dense hydrogen fluids under uniform magnetic fields. This work was performed under the auspices of the U. S. Department of Energy by the Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

4:15 PM KK5.8
Improved Electrostatics for Large-Scale Biomolecular Simulations. Celeste Sugg1, Pawel Pomorski1, Thomas Darden2 and Christopher Martin Roland1, 1Physics, NC State University, Raleigh, North Carolina; 2National Institute for Environmental and Health Sciences, Research Triangle Park, North Carolina.
Reliable biomolecular simulations are extremely difficult, because they involve complex systems such as macromolecules bathed in a solvent environment, long-range electrostatic interactions, correlation effects and a high sensitivity to both temperature and dynamical effects. In particular, an accurate and numerically efficient treatment of the classical electrostatics force fields is absolutely essential for a meaningful biomolecular simulation. Why is this? Classical codes such as AMBER or CHARMM assign a partial charge to virtually every atom in a simulation in order to model the interatomic potentials. There are two main problems associated with the current treatment of classical electrostatics: (i) how do we eliminate the artifacts associated with the point charge model; (ii) how do we efficiently simulate the very costly long-range interactions? Here, we present results on a recently developed distributed multiple method. Based on the Particle Mesh Ewald (PME) method, this formalism can treat electrostatic multipole sums to hexadecapoles without prohibitive additional computational costs. The required multipole may be effectively computed via a minimally localized Wiener filter. One of these methods for large-scale biomolecular simulations will be discussed.

4:30 PM KK5.9
We have recently developed a bond-order potential (BOP) for iridium that was found to provide not only an excellent description of cohesion in f.c.c. but also shows good transferability to more open structures as well as structures with reduced symmetry. This BOP reproduces the elastic constants and negative pressure Cauchy pressure of f.c.c. It through the introduction of a many-body repulsive term in the total energy and also yields excellent predictions for the energy of the intrinsic stacking fault and other simple crystal defects. We have applied this BOP in the atomistic simulation of dislocation core structures in f.c.c and in order to better understand plastic deformation and ultimately the origin of the brittle cleavage under tensile loading in this material. The lattice Green's function boundary conditions advanced by Woodward, Ruo and others have been implemented in our simulations during relaxation, thus enabling us to self-consistently treat the long-range strain fields induced by dislocations. The relaxed core structures of the 30°, 60° and edge dislocations have been computed and using image simulation, we
have compared the structures of the screw and 60° dislocations to 
HREM images. This research was supported the U.S. Department 
of Energy, BES Grant, no. DE-FG02-98ER45782.

SESSION KK6: Poster Session II
Tuesday Evening, December 2, 2003
8:00 PM
Exhibition Hall D (Hynes)

**KK6.1**

**Carbon Nanotubes As Mechanical Gigahertz Oscillators.**
Douglas S. Gruen*1, Sergio Legon*1, Victor Rafael Coluci*3, Scheila 
Ferrato Braga*2, Pablo Zimmerman Coura*2 and Sorrentes Oliveira 
Dantas*2.

1. Applied Physics, State University of Campinas, Campinas, 
2. Sao Paulo, Brazil; 3. Departamento de Física, UFJF, Juiz de Fora, 
Minas Gerais, Brazil.

The technological advances have led to the need of creating functional 
devices at nanometer scale. There have been continuing efforts for 
fabricating nanomechanical systems operating in high frequencies, 
but gigahertz range is beyond our present micromachining capabilities. 
A breakthough in this area has been obtained by Cummings and Zettl [1]. 
They demonstrated the controlled and reversible telescopit 
extension of multiwalled carbon nanotubes (MWNT), thus realizing 
ultrasonic friction nanoscale linear bearings. These results indicate that 
the fabrication of nanomechanical systems operating in high 
 frequencies is now a possible realization. Similarly to graphite, the 
interface interaction in MWNT is predominantly van der Waals [1], 
and since the interlayer corrugation is small it is expected that 
individual cylinders of MWNTs might easily form a stable or rotate with 
respect to one another. Depending on the distance separation between 
two adjacent nanotubes, it is possible to have an almost perfect 
sliding surface. The van der Waals interactions between the nanotubes 
create a restoring force that causes the inner tube to retract and can 
be the physical basis (and within our present technological 
capabilities) to build nanodevices [1]. 

Using static models on a slightly modified Cumbings and Zettl set up, 
Zheng et Jiang [2] have showed that multilayered nanotubes could lead to 
gigahertz nanoscale bearings. We have carried out molecular dynamics studies for these systems, 
in the framework of classical mechanics with standard molecular 
force fields [3], in order to analyze the reliability of such nanodevices and to 
determine the importance of temperature and time fluctuations. 
The calculations were carried out considering structures containing up to 
6,000 carbon atoms. Different nanotubes types (single and multiwalled 
armchair, zigzag, chiral, and combinations) were analyzed. Our results 
show that sustained oscillatory behavior is possible (for all kind of 
tube combinations) only when a perfect coupling (when the radii 
differences between inner and outer tubes are of ~ 3 Å Angstroms) 
occur. For other couplings, although the telescopit and retractive 
movements are possible, dissipative forces and momentum exchange 
among the nanotubes compromise the sustained oscillatory regime. 
Our results showed that multilayer nanotubes can be used to make 

**KK6.2**

Abstract Withdrawn

**KK6.3**

**First-Principles Calculations of Site Preference for 3d 
Ternary Elements in the NbCr2Laves Intermetallic 
Compounds.** Jian Sun*1, Bing Jing*2 and David J. Smith*3.

1. Department of Physics and Astronomy, Arizona State University, 
Tempe, Arizona; 2. Department of Physics and Astronomy, Arizona 
State University, Tempe, Arizona.

Intermetallic compounds are expected to be used as magnetic 
and magnetooptical materials and hydrogen storage materials, and, 
recently, are also considered to be potential high temperature 
structural materials. Alloy design is the most important method 
used to modify or improve the desired physical and mechanical 
properties of the Laves intermetallic compounds. Basically, altering 
alters locally the electronic structure and bond nature which, in 
turn, influences the physical and mechanical properties of materials. 
In order to identify the origin of these phenomena, it is very important 
to determine the crystalline sites of ternary elements in the Laves 
compounds. Recently, first-principles calculations have become a 
powerful tool for these purposes. In this paper, the full-potential linearized augmented plane wave method with the generalized 
gradient approximation (LAPW, GGA) has been used to calculate the 
 electronic structure and the total energy of the NbCr2Laves 
compounds. Structural stability of the NbCr2Laves compounds with the 
3d ternary elements of Ti, Mo and W, and the site preference 
energies of these ternary elements in these compounds have been 
studied systematically. The relations between the electronic structure 
and site preference of ternary elements will also be discussed. Finally, 
the calculated results will be compared with the experimental results 
of the site preference of ternary elements in the NbCr2Laves 
compounds, which obtained by atom location by electron channeling enhanced microanalysis [ALCHEM].

**KK6.4**

**Kinetic Monte Carlo Simulation of Star-Shaped Diamond 
Crystals Grown from the Vapor Phase.**
Rodrigo Chandrasekar Minz*1 and Mahendra Kumar Sunkara.*
Chemical Engineering, University of Louisville, Louisville, Kentucky.

Star-shaped crystal is one of the common five-fold twin observed in 
Diamond, as well as other crystal systems like Gallium Nitride and 
Gallium. The ratio of growth velocities in different crystallographic 
directions (as factor) has been traditionally used to explain faceting 
of diamond. This factor cannot explain the reason for 
formation of star-decagonal crystal versus a decagonal crystal, both of 
which are stable morphologies of CVD diamond bounded by [111] 
facets. We have performed Kinetic Monte Carlo (KMC) simulations 
to determine rules that govern the kinetic faceting of star-shaped 
multiply twinned crystals. In our simulations, we start with a seed 
cluster (20 atoms) and apply rules that define the site-selective 
growth chemistry for KMC scheme and grow the crystal to a certain 
size (100000 atoms). At this size, the shape of the cluster is compared 
with that observed in experimentally grown crystals. The simulations 
starting with a seed cluster containing two stacking faults, using 
growth rules that include single adsorption and desorption of single 
methyl radicals, simulate a perfect decagonal. Inclusion of 
additional step of etching atoms bonded twice to the surface allowed 
the growth of a star-decagonal cluster [1]. These simulations 
yielded the growth of star-shaped crystals, the reasons for the 
formation of kinetically stable concave [111] faces across twin 
boundaries are not clear. In this regard, we are currently performing 
simulations using detailed site-selective surface chemistry to further 
understand the reasons for formation of star morphologies versus 
perfect decagonal morphology. The results on diamond multiply 
twinned crystals could be extended to understand the growth of other 
related material systems, i.e., Gallium Nitride from molten gallium 
and Gallium nitride from gas phase. The deeper understanding of 
growth chemistry limits our ability to grow large single 

**KK6.5**

**Highly Optimised Empirical Potential for Carbon.**
Pei Gao*1, Thomas J Lenczky*2, Eric J. Bylaska*3, Anter A El-Azhari*3 and 
MS K8-60, Pacific Northwest National Laboratory, 
Richland, Washington; MT Idaho Pacific Northwest National Laboratory, 
Richland, Washington.

A highly optimized empirical potential for carbon is developed in the 
framework of modified embedded atom method (MEAM) using five 
cubic splines to describe pairwise and three-body terms, a form which 
has been successfully applied to silicon and several metallic systems. 
The potential parameters are fitted to a large ab initio database and 
experimental data using the force-matching method. The potential 
model provides a good description of energetics for all atomic 
configurations, and realistically describes interlayer forces in graphite, 
with the strain being very close to the experimental value. Phonon 
properties and elastic constants agree well with experiments and 
ab initio calculations, and smooth networks created by liquid quench 
have similar properties to the theoretical results calculated previously. 
The potential model is employed to study the structures and 
formation energies of point defects and small defect clusters in 
diamond and graphite. The predictive power of the potential 
is demonstrated in application to graphitic carbon nanotubes and 
fullerenes.

**KK6.6**

**Ab Initio Study of MoP, a New Hydrodenitrogenation 
Catalyst.** Vitor Milman*1, Bjorn Wissle*2 and Roberto 
Gonçalves*1.

1. Acropolis, Cambridge, United Kingdom; 2. Institut für Mineralogie 
Abt. Kristallographie, Johann Wolfgang Goethe-Universität, 

The structure and properties of the new catalyst, MoP, is investigated 
using plane-wave pseudopotential DFT technique as implemented in 
CASTEP program. The adsorption and hydrogenation (HDN) 
properties of propene (1,1-dipropylcyclohexane) on MoP (100) is 
chosen to analyze adsorption geometry and energetics for the 
$p\alpha$-PA molecule on the Mo(100) surface. The energy barrier for one of 
the HDN reactions ($p\alpha$-PA-propylene) is determined using the 
LST/QST transition state search method.

K.G. 10
Ideal Tensile Strength of B3 Structure 3d Transition Metal Aluminides, Toshiki Li,1,2, J. W. Morris,1,3 and D. C. Chrzan1,2,
1Department of Materials Science and Engineering, University of California, Berkeley, Berkeley, California, Materials Science Division, Lawrence Berkeley Laboratory, Berkeley, California.

The ideal tensile strength of the B3-type (CaO) transition-metal aluminides FeAl, CoAl, and NiAl have been investigated using an ab initio electronic structure total energy technique employing the local density approximation and ultrasoft pseudopotential. The ideal tensile strength is computed along the [100], [110], and [111] directions. Even though neither of these materials has identical lattice parameters and similar electronic structures in their unstressed states, they exhibit dissimilar mechanical behavior under the simulated ideal tensile tests. The ideal strength [180GPa] and corresponding critical strain [14%] of FeAl under [100] tensile is much lower than those of CoAl and NiAl. FeAl is consequently weakest in tension along [100] rather than either [110] or [111]. This behavior is in contrast to the predictions for NiAl and CoAl. Furthermore, these predictions are consistent with the experimentally observed fracture behavior for these materials. This work is supported by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Science under contract DE-AC03-76SF00098.

K.G. 11
Simulation of STM Images of Au/TiO2(110), Kanzaki Gouken1, Yasuhi Mochida2, Yoshitaka Morikawa3, Shingo Tanaka1,2, Koji Tanaka1, Masanori Kobayashi1,3,4,5. 1Department of Life Technology, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan, 2Research Institute for Computational Science (RICS), National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan.

The gold is not expected to be a good catalyst for oxidation or hydrogenation since reactive molecules such as O2 and H2 do not adsorb on gold surfaces. However, dispersed nano-size gold particle on metal oxides such as TiO2 can act as a catalyst for the room-temperature oxidation of CO and the epoxidation of propylene in a gas containing oxygen and hydrogen. To understand the mechanism of the unique activity of Au/TiO2 system, we have theoretically investigated the stable adsorption site and the electronic structures of Au/TiO2(110) based on the density functional theory. We have examined the adsorption of one Au atom on per (2 x 2) surface unit cell on three types of TiO2(110) surface condition: the perfect stoichiometric surface, the surface with the defect of the bridging-oxide, and the reconstructed 1 x 2 surface with Ti2O3 rows. We used the ab initio pseudopotential method. For the stoichiometric surface, the most stable adsorption site is the on-top site above the bridging-oxide atom and electrons transfer from Au atoms to O atoms. For the surface with the defect of the bridging-oxide atom, the most stable site is the bridging between the four-fold Ti atoms along the [001] direction, that is the bridging-oxide vacant site, and electrons transfer from Ti atoms to Au atoms. For the reconstructed 1 x 2 surface, the most stable site is the neighborhood site of the Ti atoms in the Ti2O3 rows and electrons transfer from Ti atoms to Au atoms. We have also simulated the scanning tunnel microscopy (STM) image for the three types of surfaces. We discussed the dependence of the STM images on the surface condition of TiO2(110) and the adsorption site due to be compared with the experimental results.

K.G. 12
A Monte Carlo Study of Kinetics of Precipitation in Aluminum Alloys: from Ab-Initio Calculations to Classical Nucleation Theory, Emmanuel Close1,2, Maylis Nastie2 and Christophe Sigl3, 1Prechimie Centre de Recherches de Voreppe, Voreppe, France, 2Service de Recherches de Metallurgie Physique, CEA / Saclay, Gif-sur-Yvette, France.

Zr and Sc precipitates in aluminum alloys to form the compounds Al2Zr, Al2Sc, and Al5(Zr1-xScx)2, which for low super-saturated conditions of the solid solution have the L12 structure. The aim of the present study is to model at an atomic scale this kinetics of precipitation and to link this to a mesoscopic model to be able to extend the field of super-saturations and annealing times that can be simulated. In this purpose, we use some ab-initio calculations [1,2] and experimental data to fit an Ising model describing thermodynamics of the Al-Zr/Sc system. Kinetic behavior of this
system is described by means of an atom-vacancy exchange mechanism. This allows us to simulate with a kinetic Monte Carlo algorithm kinetics of precipitation of AlZn and AlSi. These kinetics are then used to test the classical nucleation theory. In this purpose, we deduce from our atomic model an isotropic interface free energy which is consistent with the one deduced from experimental kinetics and a nucleation model. We test different mean-field approximations (Bragg-Williams approximation as well as Cluster Variation Method) for these parameters. The classical nucleation theory is coherent with the kinetic Monte Carlo simulations when CVM is used; it manages to reproduce the cluster size distribution in the metastable solid solution and its evolution as well as the steady-state nucleation rate. We find that the capillary approximation used in the classical nucleation theory works surprisingly well when compared to a direct calculation of the free energy of formation for small Li2 clusters. Acknowledgments: This work was funded by the joint research program “Precipitation” between ProInno, Unisus, CNR, and CEA. References [1] M. Asta and V. Ozolinis, Phys. Rev. B 64, 094104 (2001) [2] E. Cloquet, J. M. Sanchez, and C. Sigli, Phys. Rev. B 65, 094105 (2002).

KK6.13
Al-in situ Study of stacking in Thiophene Oligomers.
Damian Ariel Scherlis and Nicola Marzari, Materials Science and Engineering, MIT, Cambridge, Massachusetts.

Thiophene oligomers display very promising electronic and structural properties, that make them extremely attractive as building blocks for organic conducting polymers and for electrolytically conducting polymers. While a significant amount of atomic research has been carried out in the past years, there are still several issues that, while central to molecular design and engineering, remain elusive. The mechanisms of charge transport, the interaction between stacked oligomers, and the role of the solvent are all aspects that require a thorough understanding. We use here an extensive combination of quantum chemistry approaches and ab-initio molecular dynamics simulations to elucidate the stacking energetics, and to correlate it with the order of the oligomers and their different oxidation states. Moreover, we show that the presence of the solvent drastically changes the thermodynamic stability of the different dimers. Our results help rationalize the use and efficiency of novel thiophene-based materials proposed for nanotechnology applications.

KK6.14
Abstract Withdrawn

KK6.15
Simulating Pb Vacancies in Pb-based Perovskites.
Eric Goehry and Benjamin P. Burton, Ceramics Division, NIST, Gaithersburg, Maryland.

Relaxor ferroelectrics (RFE) with optimal properties for electromechanical applications are typically Pb-based perovskites. Experimental studies have revealed existence of Pb vacancies in these materials. In the present work, we have simulated the effect of Pb vacancies on the properties of Pb-containing perovskites. We studied Pb vacancies in PbTiO3 using first-principles (FP) density functional theory methods. We use the modern theory of polarization to calculate the dipole moment of the nearest-neighbor Pb-O vacancy. The dipole moment of the vacancy is greater than the dipole moment per unit cell in defect-free Pb-based perovskite ferroelectrics, which indicates that Pb-O vacancies can be an important source of local "random" fields in RFE. Finally, we use the FP results to implement a random array of Pb-O vacancies into a representative unit cell. Our model reproduces the experimentally observed temperature-dependent electric constant as a function of vacancy concentration.

SESSION KK7: Methods II
Chair: Diana Farabaugh
Wednesday Morning, December 3, 2003
Constitution A (Sherborn)

8:30 AM *KK7.1
Learn-On-The-Fly: An Adaptive Classical/Quantum Hybrid Molecular Dynamics Scheme. Giorgio Ciccotti, Enrico Tosatti, Mike C. Payne and Alessandro de Vita, Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom.

An embedded molecular dynamics scheme is presented which spans the lengthscale gap between feaseable classical and quantum mechanical computer simulations. It is ideal for problems in which only a small fraction of the atoms need to be treated quantum mechanically, yet a large number of atoms is explicitly required to correctly represent the geometry and the elastic properties. The method facilitates automatic selection of quantum regions and uses force matching to continuously and gradually modify the classical potential to resemble quantum trajectories. The correctness of macroscopic observables is demonstrated using native defects of silicon. A simulation of brittle fracture in silicon reproduces the main experimental features using a hundred thousand classical atoms and a few thousand atoms in the tight binding approximation near the crack tip.

9:00 AM KK7.2
Feature Activated Molecular Dynamics for Accessing Large Length Scales. Marish Prasad and Tadi Simo, Department of Chemical Engineering, University of Pennsylvania, Philadelphia, Pennsylvania.

An increasingly important goal in materials process modeling is the incorporation of atomistic information to create physically realistic models at larger scales. Efforts to couple disparate length and time scales have relied either on concurrent or sequential approaches, based on the physics of the problem. In the former, where length scales cannot be completely decoupled, the challenge is to seamlessly connect multiple representations together into a single simulation. These frameworks can greatly leverage the scope of an atomistic simulation, without necessitating that complex atomistic phenomena, such as defect segregation in solids, be coarse-grained. A new hybrid scheme based on molecular dynamics (MD) suitable for modeling the evolution of atomic defects and their aggregates in solid-state materials is described here. Such species are typically present in very dilute quantities in crystalline solids, and their effects on the surrounding lattice are usually small. These defects, however, are not fixed and can evolve dynamically by the systematic "turning-on" and "turning-off" of atomic thermal excitation (activity). This approach provides for "seamless" activation and deactivation of lattice atoms in the presence of defect diffusion, aggregation and fragmentation. This is achieved by placing a thermal envelope around the individual defects. The envelope function determines the size of active region and the activity of atoms in the system. The hybrid MD approach is tested and validated by comparison to regular MD predictions of transport and formation properties of vacancies and small clusters in crystalline silicon. Next, the predictions of a large-scale hybrid system are compared with previous MD results for the vacancy aggregation problem involving a lattice of 215,000 Si atoms and 1,000 vacancies is evolved in the NVT ensemble at 1600 K. These comparisons establish that the hybrid MD scheme with multiple dynamical regions is equivalent to a regular MD simulation. The computational performance of the schemes is compared for different system sizes and defect concentrations. It is shown that the computational time per MD step is essentially independent, for a given number of defects, from the actual size of simulation system, making it suitable for modeling of very dilute systems. The overhead involved in doing additional identification/propagation of active and static regions is also negligible.

9:15 AM KK7.3
Adaptive Importance Sampling of Rare Transition Events. Maurice de Koning 1,2, Wei Cai, Babak Sadigh 2, Mathi H Kalos 1 and Vasily V Bulatov 1, 2 Lawrence Livermore National Laboratory, Livermore, California, 1 Instituto de Fisica, DPFM, Universidade de Sao Paulo, Sao Paulo, SP, Brazil.

We present a new approach to the simulation of rare transition events using Importance Sampling Monte Carlo framework. The approach approaches the problem by enhancing the probability of sampling sequences of states, or paths, that constitute successful transition events between two metastable states. This is accomplished by means of an Importance Function, which modifies the transition probabilities of the original unbiased Monte Carlo dynamics. In addition to preserving the relative sampling probability of different successful transition paths, the approach enhances the probability of sampling a successful transition event by a known amount, facilitating the evaluation of transition rates. In this manner, the rare-event problem is transformed into an optimization problem, that of finding the best-possible Importance Function for the transition at hand. We developed an adaptive algorithm that iteratively adjusts the Importance Function until satisfactory efficiency is achieved. The method is demonstrated on low-dimensional model problems, as well as on a realistic atomistic system of dislocation motion in silicon. Computational with other existing methods. The work was performed under the auspices of the U. S. Department of Energy.
by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48. MK acknowledges support from the Brazilian agency FAPESP.

9:30 AM KK7.4
A novel, fast and reliable accelerated molecular dynamics method: theory and applications. Francesco Montemezzi1, Blue P. Uheruga1,2, Gregoire Henkelman2 and Arthur F. Voter1,2. 1Materials Science Department, University of Milano, Milano, Italy; 2Theoretical division, Los Alamos National Laboratory, Los Alamos, New Mexico.

In fundamental surface phenomena such as crystal growth and island diffusion, experimentally relevant time scales are of the orders of seconds or longer, while numerical orders of magnitude longer than the typical time scale achievable by traditional molecular dynamics simulations. Accelerated molecular dynamics techniques [1] provide a useful tool to close this gap substantially. In this work we show that two methods have very different philosophies, and we compare them to obtain a fast and reliable accelerated molecular dynamics technique, dimer-TAD. In dimer-TAD, the dynamics out of a state is described using the temperature-accelerated dynamics (TAD) method [2,3], enhanced by the knowledge of the minimum barrier out of the state coming from a set of dimer-method [4] saddle searches. As an application of the method, we simulate diffusion of islands of various sizes on (100) metal surfaces, reaching time scales of seconds at T=900 K. A complex diffusion scenario is revealed, where multi-atoms mechanisms play a key role in determining island shape and mobility.

10:15 AM KK7.5
A Nose-Ponteaction Quasicontinuum Model. Laurent Michel Dupuy and Rob Phillips; Mechanical Engineering, California Institute of Technology, Pasadena, California.

In this paper, we extend the quasicontinuum method to study the dynamical properties of defects in metals at finite temperature. The Nose-Ponteaction method is a technique to perform deterministic and Hamiltonian molecular dynamics at constant temperature. Here we present a derivation of this method to perform simulations in a mixed atomistic and continuum setting through the use of coarse-grained potentials. In this way, the number of degrees of freedom is significantly reduced allowing to simulate systems on relatively small computers. Although the behavior of all the atoms is not considered, it is shown that the equilibrium properties of a full atomistic system in the canonical ensemble are recovered. The validity of the proposed method is demonstrated by computing thermal properties of a defect-free single crystal.

10:30 AM *KK7.6
Prediction of Nanostructural Evolution Based on First Principles*. Zheng Zhang, 1Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; 2Department of Physics, Univ. of Tennessee, Knoxville, Tennessee.


11:00 AM KK7.7
An improved ELMC method for simulating atomic layer deposition of metals. Michael Mueller and Kirsten Albe; Institute of Materials Science, TU Darmstadt, Darmstadt, Germany.

We present an improved kinetic Monte Carlo scheme for modeling layer deposition of metal that not only describes single atom jumps, but also cluster diffusion on surfaces. Regular lattice sites as well as stacking fault positions are included and a new EAM-based coating scheme is used for calculating activation barriers during the simulation run. The method is applied to simulate sub-monolayer growth of Ir on Ir[111], where we achieve very good agreement of calculated island distributions and island shapes with results from STM-measurements.

11:15 AM KK7.8
Atomatic Model of Polycrystalline Thin Film Evolution under Stress. Hinchen Huang1, 2; George Gilmer2, 2; L. G. Zhou1, 2; Timothy Cale1, 2. 1Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, New York; 2Materials Science and Technology, Lawrence Livermore National Laboratory, Livermore, California; 3Department of Chemical Engineering, Rensselaer Polytechnic Institute, Troy, New York.

Texture is pivotal to the performance of thin films, and its nucleation and evolution are a direct result of atomistics processes. Complementing characterizations experiments, atomistic modeling and simulations are helpful or essential in achieving the optimal texture. Our atomistic model ABP-TBDP has been implemented to simulate nucleation and evolution of two textures at the atomic level and under realistic deposition rates. In this work, we present the implementation of multiple-texture model. The spatial positions of atoms are represented accurately within one atomic diameter, naturally enforcing an accurate representation of atomic density averaged over one unit cell. The model is tested on a model system: copper. Atomic energetics of copper are used in the ADEPT simulations, and the results serve the purpose of both model validation and interpretation of our experiments on copper texture evolution.

11:30 AM KK7.9
Application of the NRL Tight-Binding Model to FCC Metal Surfaces. Michael I. Hafel, Naomi Bernstein, Michael J Mehl and Dimitris A Papasimakis; Center for Computational Materiak Science, Naval Research Laboratory, Washington, District of Columbia.

We employ the NRL tight binding (TB) model to predict the interlayer surface relaxations and surface energies for the low-index faces of Cu, Ni, Pd, Rh. We compare the TB calculations, utilizing self-consistent charge transfer, with experimental measurements, density functional theory (DFT) calculations, and semiempirical methods. We find that for these metals, the TB model reduces the DFT surface-exposed fcc surfaces, whereas the full self-consistent calculations either predict small expansions or contractions. We also examine the energetics and relaxations of the (111) missing row reconstruction for these metals. The NRL-TB model predicts that Pd and Pt undergo this reconstruction, while Ir, Ni, Pd, and Rh do not, whereas experimentally this reconstruction is observed for Pt, Au and Ir. The interatomic relaxations of the (111) missing row structure for Pt, Au and Ir are in good agreement with DFT calculations and experiment.

11:45 AM KK7.10
Atomic Simulations of Hydrocarbon Decomposition on Metal Surfaces Induced by a Sliding Diamond Tip. Stacie LeSure Gregory, Kui Wang and Donald W. Brenner; Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina.

Nanoscopic devices containing moving components have been envisioned for applications that include energy storage, chemical sensing, and thermal-based heat management. The operation of these devices requires the ability to perform solid-state surface science experiments at ultra-fast rates. We have developed a new technique, termed ‘nano-scanning-tunneling mass spectroscopy’ (nanoSTM-MS), to perform ultra-fast atomic level experiments on a nanoscopic scale. We will present measurements of the fate of hydrocarbon decomposition on a nanoscale sliding system. Initial experiments predict that chemisorbed monolayer is more robust than that on sub-monolayer sliding conditions on nickel [111] surface.
Superalloy: A Kinetic Monte Carlo Simulation Study, Zuyang Mao,1, George Martin2,1 and David N. Seidman3,1 Materials Science & Engineering, Northwestern University, Evanston, New York; Service de Recherches en Metallurgie Physique, Centre des Etudes Atome, Sacy, France.

The diffusivities in Ni, of Al or Cr solute atoms and clusters of these solute atoms, dimers through sextets, are studied utilizing three-dimensional kinetic Monte Carlo (KMC) simulations; the parameters employed are compatible with existing thermodynamic and diffusion data for this ternary alloy. We demonstrate that, in Ni-873 K, the diffusivities of Al or Cr clusters (dimers, trimers, quadruplets, and pentamers) or mixed Al-Cr clusters are greater than the diffusivity of a single Al or Cr atom in Ni, where diffusion occurs via a macroscopic mechanism. The presence of macroscopic-solute atoms is the origin of this fast diffusion of clusters, which is a consequence of long-range solute-solute interactions. They are suppressed by introducing chemical potential interactions that alter neither the thermodinamics nor the macroscopic diffusion coefficients of the alloy. Furthermore the temporal evolution of the nanostructure of a Ni-5.2 Al-14.2 Cr alloy model superalloy is studied both with and without vacancy-solute interactions. With vacancy-solute interactions about 40% of the gamma prime precipitates are interconnected by necks after an aging time of about four hours, whereas without solute-vacancy interactions the necks are completely absent. These results are compared to recent three-dimensional atom probe (3DAP) microscopy experiments being performed at Northwestern University on the same alloy (Studbrink, Yoon, Isbreh, Mao, Noebe, Seidman, 2003), and it is shown that the detailed experimental observations of gamma prime precipitates in the gamma matrix, as a function of aging time, are in semi-quantitative agreement with our computational results. This implies that the coarsening mechanism of the gamma prime precipitates in this alloy most likely occurs by a cluster-diffusion-competition mechanism and not by the classical mechanism, which involves the evaporation of a single atom (monomer) from a shrinking precipitate and its condensation on a growing precipitate. Research supported by the National Science Foundation (K. L. Murry, grant officer).

2:30 PM KBS.4 Pipe diffusion of Mg in a binary Al-Mg alloy, Canlin Piao and David Zhang, Renault-Polytechnic Institute, Troy, New York.

Solute diffusion in an Al rich binary Al-Mg alloy is studied by means of atomistic simulations. The activation energy for diffusion of Mg in the bulk is evaluated in the dilute solution limit for the nearest neighbor and the ring mechanisms. Further, diffusion of Mg along the core of edge, 690 and screw dislocations is studied. It is observed that, similar to the bulk, Mg diffusion in absence of vacancies is energetically prohibitive at room temperature. The paths of maximum activation energy are identified for vacancy-assisted diffusion, for all three types of dislocations. Most diffusion paths have activation energies larger than 75% of the equivalent bulk quantity. This analysis is relevant for the discussion on the microstructure diffusion of dynamic strain aging in these alloys. The data presented here show that pipe diffusion, which is currently considered as the leading mechanism responsible for dynamic strain aging and the Portevin-Le Chatelier effect is too slow to account for the observed mechanical behavior under most experimental conditions.

2:45 PM KBS.5 First Principles Calculation of Diffusion in Binary Alloys. Anton Van der Ven and Gerbrand Ceder, Materials Science, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Diffusion in multicomponent solids plays an important role in battery and fuel cell applications as well as during the synthesis of a material as this is often accompanied by phase transformations involving atomic redistribution. We have extended the tool of alloy theory (theory of first principles phase diagrams) to study of diffusion in solids with configurational disorder. We have applied this formalism to study diffusion in Al-Li alloys as a function of alloy composition and temperature from first principles. We predict that the vacancy concentration in this alloy has a strong dependence on the short-range order among lithium and aluminum atoms with the vacancy preferring aluminum over lithium in its first nearest neighbor shell. Furthermore, the vacancy concentration is predicted to depend strongly on alloy composition within this ordered ABII L12 phase. While the vacancy prefers aluminum rich environments, first principles calculations of activation barriers predict that Li has a low activation barrier that the Al-Li exchange is the neighboring vacant site. With the cluster expansion formalism combined with kinetic Monte Carlo simulations, we have calculated the alloy diffusion coefficient using Green-Kubo relations. Together with first principles free energy curves, the calculated diffusion coefficient can be used in phase-field models to predict the kinetics of precipitation transformations in this alloy.
3:30 PM #K8.6

Langevin Molecular Dynamics Simulations of Self-Assembly of Tethered Nano Building Blocks, Sharon C Glotzer1,2, Elfie R. Chen1, Mark A Horsley1, Monica H Lamm1, Charles (Xi) Zhang2 and Zhenli Zheng2, 1Department of Chemical Engineering, University of Michigan, Ann Arbor, Michigan, 2Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan.

The application of nanotechnology to areas such as photonics and electronics requires that nanoscale objects such as nanoparticles and nanostructured molecules interact in a functional manner and device. Currently, few demonstrated assembly approaches offer a comprehensive, systematic, and generally applicable scheme for the rational assembly of nanoparticles into one-, two-, and three-dimensional ordered structures. Inspired by recent advances in synthesis and functionalization, we seek to develop an intuitive framework for the assembly of nanoparticles functionalized with organic tethers. Simulation offers a unique opportunity in this regard, provided appropriate models can be devised and the length and time scales relevant to the assembly process can be efficiently accessed. In this talk, we present new results of Brownian dynamics (Langevin MD) simulations of tethered nanocrystals and polyhedral oligomeric silsesquioxanes and their self-assembly into complex ordered structures. We show how tuning thermodynamic parameters and architectural features of model nano building blocks can control aspects of local and global ordering of the nanoparticles. We further demonstrate that for certain categories of tethered nano building blocks the morphologies obtained may be predicted using concepts from block-copolymer micellization and self-assembly of nanoparticles/tether topology leading to structures richer than those found in conventional block copolymer, surfactant, and liquid crystal systems, including nanowires, nanoshells, and nano-cylinders. This work is supported by grants from the National Science Foundation (DMR 0102337 and DMR 0210551) and the U.S. Department of Energy (DE-FG02-02ER04090).

4:00 PM KK8.7

Design and testing of dendrimer templates using structural and functional analysis by new cross-linking methods, Hiroshi Tako, Tahir Cagin and William A Goddard, Material and Process Simulation Center, Beckman Institute [13a-74], Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California.

A new computational scheme was developed to create cross-linked structures of polymers from reactive molecules. This scheme uses a combination of Monte-Carlo (MC) and Molecular Dynamics (MD). Each cross-linking step has a separate MC and MD components. The MC part provides several structures with one new cross-link. The MD part evaluates the total energy for these structures, and selects the lowest energy structure as the continuous growing direction. These MC/MD calculations are repeated to find the final multiply cross-linked molecular structure. This scheme was applied to predict the structure of cross-linked dendrimers composed of PMMA and Silic acid of the University of Illinois [ref1]. Their dendrimer used a core and resulted in multiple allyl-functions, one at the end group of each dendron. These alkyl functions were cross linked using a Grafted Rod-like ring-closing metathesis catalyst. This dendrimer contained 64 allyl-functions, so that the maximum number of cross-links was 32. The experiment detected 29 cross-links. We developed 30 independent cross linked structures, leading to 24 to 31 cross-links with an average of 28 cross-links, in good agreement with experiments. We find that 60% of the cross-links are inter-dendron. After creating the cross-links the experiments eliminate the porphyrin core by hydrolysis, and found that the core dendrimer was selected as the specific heptamer. We make the same calculations with the computational core Dendrimers and find results similar to the experiment. This indicates that such simulations might be useful in designing new dendrimer template systems, ref1 Stefan Z. Zimmerman, et al NATURE Vol.418 (819), 25 July 2002.

4:15 PM #K8.8


Here we demonstrate a procedure for modeling the conformational instability of switchable molecular devices. In this procedure, full-torsion angle conformational search based on empirical molecular modeling is first carried out to generate a large ensemble of chemically reasonable conformations. Next, lower-level electronic structure calculations are performed for all conformations to identify the most significant structures. Higher-level electronic structure calculations are then carried out for a subset of conformations. This is followed by statistical analysis of the results to correlate structural features to energy. We have applied this procedure to two prototype molecular devices in order to investigate their switching mechanisms and multiple stability: (I) an electrochemically-switchable [2]catenate and (II) a photo-switchable quaterthiophene-substituted azobenzene. For system (I), the procedure yields structural preferences that are in excellent agreement with previous studies for both the single and double states. For system (II), again the computations recover the experimentally observed structure/energy profile, showing that the structures with a trans-azobenzene configuration are more extended and have lower energy than those with the cis-azobenzene configuration. We propose that the procedure has promise for use as a molecular design tool.

4:30 PM #K8.9

Pore Structure and Physical Properties of Simulated Silica Gels, Sudip Bhattacharya, Liping Huang and John Kieffer, Material Science and Engineering, University of Michigan, Ann Arbor, Michigan.

Molecular dynamics simulations based on a recently developed charge-transfer three-body potential were used to generate nano-porous silicon gel structures. In these simulations care was taken to reproduce the sol-gel condensation reaction that lead to the gel backbone as realistically as possible and to thereby produce credible gel structures. By varying the reaction conditions different gel structures were created, from which obtained by simulated annealing were then examined to reveal the relationship between the structure and properties. Structural analysis was carried out in terms of geometric and dimensional correlations. Thermal and mechanical properties were derived from the vibrational density of states obtained through normal mode analysis. In this presentation we will report our findings and discuss how the non-Euclidean dimensionality of the gel structure affects its vibrational behavior and any derivative properties.

4:45 PM #K8.10

Understanding medium-range order of amorphous systems under high pressure: numerical simulations, Lilian P Davila1,2, Marisa-Jose Cazuela2,3, Alfonso Kubat1, Babak Sadigh4, Tomás Díez de la Rubin5, James F. Shuckelford5, Subhash H. Rando6 and Stephen H. Groenfalk7, 1Dept. of Chemical Engineering & Materials Science, UC Davis, Davis, California, Lawrence Livermore National Laboratory, Livermore, California; 2Dept. of Physics, University of Alicante, Alicante, E-03607, Spain; 3Dept. of Ceramics and Materials Engineering, Rutgers University, Piscataway, New Jersey.

Structural transformations of the medium-range order and the dynamic behavior of silica glass at high pressures is still not well understood despite years of research. Recent papers have shown how the medium-range order can be used to guide experiments resulting in materials of scientific and technological interest. We have used MD simulations to study the behavior of fused silica under pressure using empirical interatomic potentials constructed by Freidzon and Groenfalk. In this article we present two different simulation schemes for studying the structural transformations in fused silica under high pressures, and show their equivalence. Both methods reproduce the equation of state (EOS) obtained from flyer plate experiments. We have centered our studies in the structural changes occurring in the material with increasing pressure and the correlation between the medium-range order, through the structure factor, and the characteristic ring distribution of these amorphous glasses. An analysis of the ring distribution and structure factor reveals the microscopic changes occurring in this material and allows for an interpretation of the equation of state. The transition from elastic and plastic behavior is direct with structural variations exhibited in the ring size distribution of this glass. During elastic compression, the ring distribution stays practically unchanged. However, this transition varies continuously after the transition to the plastic regime takes place. This study can help understand the nature of fused silica, influencing applications that depend on its structure under these conditions with implications in geophysics, glass technology and optics. This work was performed under the auspices of the U.S. Department of Energy with experiments at the Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

SESSION K89: Poster Session III

Wednesday Evening, December 3, 2003

8:00 PM

Exhibition Hall D (Hynes)

E1K9.1 Investigation on Filling of (10,10) Single-Walled Carbon
CUNY, Brooklyn, New York.

Knowledge of the nature and properties of the grain boundaries (GBs) in YBCO is of primary importance for the development of high-Tc cables and tapes, as well as Josephson devices. Different mechanisms have been suggested to explain the influence of GBs on superconducting properties of YBCO. Chiasholm and Pennycook [M. F. Chiasholm and S. J. Pennycook, Nature, 351, p. 47, 1981] suggested that superconductivity at GBs suppressed by strain. For the large-angle GBs, the dislocation model of GBs becomes inapplicable and the strain field of GBs cannot be analytically calculated. The only reliable method of determining it is by direct modeling, using appropriate interatomic potential and simulation techniques. The goal of this paper is to evaluate the influence of GB structure of GBs (presence of point defects and changes) on the suppression of superconductivity at GBs. The atomic structure of large-angle symmetric tilt GBs [m(100) and 3(113)] with neutral and charged oxygen vacancies in YBCO is studied by computer simulation. As [V. S. Boyko and A. M. Levine, Phys. Rev. B, 64, p. 224525, 2001], we apply to the obtained atomic structures the techniques of bond-continuum-sum analysis [N. D. Browning et al., Phys. Rev. C, 294, p. 180, 1989] and strain analysis [V. S. Boyko, J. Malinsky, N. Abdellatif, and V. V. Boyko, Phys. Lett. A, 234, p. 56, 1998] to determine the thickness of nonsuperconducting layers enclosing GBs and evaluate their transport properties. The two methods bring outcomes that are consistent with each other. Based on our results we can conclude that the presence of oxygen vacancies may improve (at least at some concentrations) transport properties of large-angle GBs in YBCO. Experiments [M. A. Nascimento et al., Phys. Rev. Lett., 76, p. 1326, 1996; Phys. Rev. B, 50, p. 7876, 1994] demonstrated that the introduction of GBs in YBCO results in the appearance of oxygen vacans, as well as increasing Jc. Our computer simulation data might be considered as a possible explanation of these experimental observations.

K10.5 Bridging atomic and continuum scales for modeling stress defects: the importance of supercell size. Mathieu Bouville 1, Michael L. Falk 2, and Krishna Garikipati 2.

1Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan.
2Department of Mechanical Engineering, University of Michigan, Ann Arbor, Michigan.

Vacancies in silicen undergo an elastic relaxation that contributes to the formation energy of the defect. This elastic relaxation also couples the defect energy to an externally applied stress. Understanding the coupling is important for modeling the effects of stress on microstructure and predicting mass transport in the crystal. Formation volumes and energies are generally obtained using ab initio methods as only they can take into account the quantum mechanical effects that dominate close to the vacancy. However, ab initio simulations use relatively small supercells (a few hundreds of atoms), which can lead to strong vacancy-vacancy interactions with periodic boundary imps the results. Empirical potentials that are well tested are not accurate close to the vacancy but they allow for larger simulations and are therefore useful for exploring the effects of the system size on simulation results. Using molecular dynamics (MD) in Stillinger-Weber silicon and continuum elasticity we show that periodic boundaries can interfere with the calculation of the formation volume. More precisely we study how the system size affects the relaxation both at the defect and close to the boundaries of the supercell. These empirical calculations can improve the accuracy of ab initio calculations by providing an accurate estimate of the error that results from the small supercell. The relative importance of elasticity and atom-scale effects will be discussed.


Crack propagation studies in nanocrystalline -iron samples with grain sizes ranging from 6 to 12 μm are reported at temperatures ranging from 100K to 600K using atomic simlations: an empirical many-body potentials. The mechanisms of plastic deformation energy release are studied in detail. Intergranular fracture is shown to proceed by the coalescence of nano-voids formed at the grain boundaries ahead of the crack. The simulations also show that an atomistic scale fracture resistance and plastic deformation energy release mechanisms increase with increasing temperature. The infuence of carbon impurities present on the grain boundaries is studied and our results show the presence of C impurities increase fracture resistance.


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Science and Engineering, University of Utah, Salt Lake City, Utah;
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We perform extensive first-principles calculations to elucidate the topographical atomic-force-microscope image of an adsorbate on the Si(111)-7×7 surface, demonstrating the feasibility of imaging not only the atoms but also the atomic orbitals. Our comparative study of tip terminations shows that two atomic features can appear for a single adsorbate when it is imaged by a Si(111) tip having two different terminating lattice vectors, while only one feature is seen when it is imaged by a Si(111)-1 type tip having one dangling bond on the apex. The key condition for seeing the atomic orbitals is to bring the tip so close to the surface that the magnetic dependence dominates the tip-surface interaction. This work is partially supported by DOE.

**K9.8**

**Simulating Surface Diffusion and Surface Growth in Ceramics.** Duncan J. Harris 1, Mikhail Lavrenteva 1, John H. Herring 1, Neil L. Allen 1, and John A. Parson 2.

1Physics and Astronomy, University College London, London, United Kingdom; 2Chemistry, University of Bristol, Bristol, United Kingdom.

**Synopsis:** Radiation, CCLRC Daresbury Laboratory, Warrington, Cheshire, United Kingdom.

Attempts to simulate surface diffusion and growth in ceramics often run into problems of timescales. It is not possible to run a molecular dynamics simulation for long enough to reach the timescales set by, for example, Molecular Beam Epitaxy. We demonstrate that a combination of the temperature-assisted hyperdynamics scheme of Voter and coworkers with Kinetic Monte Carlo can reach these timescales required while retaining an unbiased selection of the diffusion processes. Our computer simulations show that exchange processes dominate ionic surface diffusion on terraces in ceramics. However, the process differs essentially from surface exchange diffusion in metals because the Coulombic bonding between ions ensures that the ions must diffuse in pairs. The ion-ionic interaction therefore moves across the surface by alternate exchanges of the cation and anion with the corresponding ions in the surface while the counterions remain close by, held by Coulombic attraction. Diffusion along steps is also an exchange process, except now the ion of the molecule therefore moves across the surface by alternate exchanges of the cation and anion at the edge of the terrace. We also present results for hetero-interfaces and ternary systems. Here the different lattice parameters of the ionic molecule and substrate and the different Meludung potentials in the substrate greatly complicate the diffusion behaviour. We also discuss the important issue of whether it is possible to grow atomically sharp interfaces in ceramic hetero-interfaces, or whether the exchange mechanism makes mixing unavoidable.

**K9.9**

**Ab Initio Study of the Structural Stability and Magnetic Properties in the Immiscible Co–Ag and Fe–Cu Systems.** I.T. Kong, F.J. Gong, and T. Jin Liu; Dept. Mat. Sc.& Eng., Tsinghua University, Beijing, China.

The structural stabilities and the magnetic properties of some possible metastable alloys and equilibrium immiscible Co–Ag and Fe–Cu systems were studied by ab initio calculations based on the projector augmented wave (PAW) pseudopotentials [1, 2]. Ab initio calculations first identify that the metastable fcc and bcc structured Co are both magnetic with a larger magnetic moment than the equilibrium bcc Co. For the Co–Ag system, calculations reveal that the ferromagnetic states of the D1h_3, D1h_1, and B2 structures are energetically favored for the CoAg, CoAg_2, and CoAg_3 alloys, respectively. Experimentally, a D1h_3 CoAg alloy has ever been obtained, thus supporting the ab initio calculations. From the calculation results, it seems to suggest that the magnetic moments of Co tend to be enhanced by an expansion of its average atomic volume, yet reduced by the alloying of the non-magnetic element of Ag [3]. While in the Fe–Cu system, calculations reveal that both for structured CuFe and CuFe alloys are ferromagnetic and the Cu alloying probably plays a role in stabilizing the fcc Fe, which is frequently noted surface anti-ferromagnetic, in a ferromagnetic state. Interestingly, the above calculation results agreed well with the retrieved experimental observations [4]. Reference: 1. G. Kresse and D. Joubert, Phys. Rev. B 59, 1758 (1999). 2. J.J. Liu, Z.C Li, B.N. Liu, G. Kresse, and J. Hafner, Phys. Rev. B 63, 155201 (2001). 3. T. Kong, R.F. Zhang, Z.C. Li, and B.X. Liu, Phys. Rev. B, (to be published). 4. A. Miskulnapad, B.K. Pandolfs, A.R. Srivastava, A. Gupta, K.G.M. Nair, R.V. Nandasor and A. Narsimhan, J. Phys. Condens. Matter 14, L641 (2002).

**K10.0**

**Water Interaction with Polar Semiconductor Surfaces: The Case of SiC(001).** Alessandra Carella,1 Giancarlo Cicero,1,2 and Giulia Galli,1,3.

1CNLMEMFIM, University of Firenze, Italy; 2INFN & Torino Polytechnic, Torino, Italy; 3Lawrence Livermore National Laboratory, Livermore, California.

The study of water adsorption on surfaces is an essential prerequisite for understanding the initial stages of wet oxidation processes. Furthermore, the characterization of the interface between water and semiconductor surfaces is key for the design of suitable devices operating in biological ambient. Here we present the investigation of a prototype water-like capable surface: H2O on SiC. Using first principles simulations we have studied the adsorption of water molecules on SiC(001) surface. Our results indicate that these polar SiC surfaces closely resemble their respective common Si and C counterparts. Implications for surface functionalization are outlined.

**K10.11**

**Molecular Simulation of the Mechanical Properties of a Model POSS/Polymer Nanocomposite.** Franco, M Capacci,1

1Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; 2Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Polyhedral Oligomeric Silylsequioxanes (POSS) consist of a roughly spherical inorganic silicon-oxygen framework with pendant organic groups promoting compatibility of the particles with the polymer matrix. The resulting nanocomposites have been shown to exhibit increased thermal stability, enhanced stiffness, and toughness. Significantly, some POSS nanocomposites exhibit reduced melt viscosity while exhibiting a higher Tg and an increased stiffness below Tg. Using parameters determined from molecular simulation, we find that simple continuum models fail to capture the behavior in the modulus of these nanocomposites. In order to determine the reasons for the failure of continuum theory, the mechanical properties of a model elastomer/POSS nanocomposite with perfectly dispersed POSS particles are determined through molecular dynamics simulation. The influence of the type of organic pendant group and the length of tether connecting the POSS cage to the chain backbone on the polymer chain dynamics, modulus, and structure are also investigated.

**K10.12**

**Molecular Dynamics Simulations of Velocity Distribution and Local Temperature Changes During Rapid Cooling Processes in Excimer-Laser Annealed Silicon.** Byoung Min Lee, S. Munetoh and T. Motoki; Dept. of Materials Science and Engineering, Kyushu University, Fukuoka, Kyushu, Japan.

Thin-film transistors fabricated from Si films deposited on glass substrate can perform in a number of applications such as active-matrix liquid-crystal displays and CMOS devices. In order to improve the device performance, high-quality poly-Si films with large grain sizes are required. However, since it is experimentally difficult to observe directly the crystal growth behavior, the detail of Si thin film growth is not well understood in atomic scale. In this work, we have performed molecular dynamics simulations to capture the atomic-scale local temperature changes of the system during rapid cooling processes in excimer-laser annealed Si. A MD cell with typical size of 48.87×48.87×97.75Å including 11694 Si atoms was used for simulations. The interatomic forces were calculated using the Tersoff potential and atomic motions were determined by solving Langevin and Newtonian equations by assuming that the temperatures at the substrate and surface are 1500K and 300K, respectively. The velocity distributions in melted Si during rapid cooling processes were found to be the Maxwell-Boltzmann type and steady-state temperature distribution was obtained between the substrate and surface in 110ps. The dynamical behavior of Si during rapid cooling processes was also studied.

**K10.15**

**Combining Theoretical and Experimental Evidence for Carbon-Vacancy Binding in Austenitic Steels.** Ronald Ghibali1 and Christopher Wolferton 2.

1Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan; 2Scientific Research Laboratory, Ford Motor Company, Dearborn, Michigan.

We have performed first-principles gradient-corrected density functional calculations to binding energy of nearest-neighbor carbon-vacancy pairs in face-centered cubic iron (austenite). A value of 36 kJ/mol is obtained. This result is compared to values obtained or implied from several sources of experimental data on austenite alloys, and generally good agreement is found. Experimental data examined include: point-defect metastability, self diffusion, high-temperature steady-state creep, strain aging and
strain-age hardening, and radiation damage. Several other stability calculations, primarily for metastable carbides, in the Fe-C alloys will be reported.

**KK0.14**

**Electronic Structure of Silicon Nanocrystals with Metallic Contacts.** Anna Maria Mazzoni, Istituto IIM, CNR, Bologna, Italy.

The intensive efforts conveyed in these years on transport properties of electronic devices with nanoscale dimensions have finally made clear that the electronic transport critically depends on the overall performance of the device and the theoretical progress in this field lags behind the technological advancement. Considered the many applications of nanocrystalline silicon for electronic, optical and photovoltaic devices the focus of this contribution is on the effects of metallic contacts on silicon nanostructures and the study is performed using quant'mechnical calculations at semi-empirical level, based on the MNDO approach, and LDA with pseudopotentials and LCAO wavefunctions. The size and shape of the nanocrystals realistically compare with the ones of standard nanocrystalline technology. The results of an extensive investigation on the functional dependence of the electronic configuration of the system on the size and shape of the nanocrystals, on the composition (Al, Ti, and N), and geometry of the contacts, as well as the LDA functional, are presented. The study is complemented by an analysis of the results in the light of the Boltzmann transport equation.

**KK0.15**

**Trends in native-defect enhanced diffusion of acceptors in silicon.** Giorgio M. Lopez1, Claudio Mela2, Paolo Schiavin1, Paola Alippi2 and Vincenzo Ferranti1.

We study from first principles within density functional theory trends in the energetics and migration properties of the B, Al, Ga, and In acceptors and their complexes with Si self-interstitials and vacancies in Si. Native-defect-enhanced diffusion is found to be preferred in all cases over "stuck-atom" diffusion. Non-trivial anharmonicities both in vacancy- and interstitial-mediated motion are identified, among which e.g. having zero vacancy-exchange barrier, and unstable second-neighbour Si vacancy, the Ga-In complex being metastable against transformation into a Ga Ti interstitial the capture radius being 3rd, 3rd, and beyond 4th neighbours for Ga, In, and B respectively. Observable consequences for diffusion are discussed.

**KK0.16**

**Virtual Fabrication of Electronic Nanomaterials of Prescribed Charge Transport Properties.** Lia Lakis, A. Pazar, McGill, Air Force Research Laboratory, Wright-Patterson Air Force Base, Ohio.

The focus of this presentation is on further advances in theoretical and computational methods to investigate prospects of effectively three-dimensional fabrication of sub-100 nm nanostructured electronic materials (e.g., quantum dot devices, artificial atoms, etc.) in terms of the equilibrium two-dimensional material fabrication. The desired physical properties in particular, conductivity) of such materials are achieved using predictions of the discussed fundamental quantum-theoretical approach in synergy with the equilibrium quantum statistical mechanical computations and simulations. The developed approach furnishes explicit expressions for the technological conductivity, dielectric and magnetic susceptibilities of spatially inhomogeneous systems (such as semiconductor quantum dots, artificial atoms, etc.), in terms of the equilibrium two-dimensional temperature Green functions that reflect electronic structure of the systems. These Green functions can be approximated theoretically or recovered computationally. The latter case opens rich opportunities for the simulation of synthetic devices and systems by design.

**KK0.17**

**Formation Pathways for Single Wall Carbon Nanotube Multiterminal Junctions.** Inna Ponomarenko, A. N. Andriotis2 and M. Menon.

The carbon nanotube junctions have recently emerged as excellent candidates for use as building blocks in the formation of nanoscale electronic devices. In particular, in a three-terminal junction, the third terminal could be used for controlling the switching mechanism, power gain, or other transistors applications that are needed in many other electronic devices. Recent experimental and works have demonstrated the feasibility of using controlled electron irradiation in tailoring the junction geometry to create desired multiterminal junctions of carbon nanotubes. Using tight-binding molecular dynamics simulations we illustrate the formation of simple wall carbon nanotube T, Y, and X-junctions through an energetically efficient pathway in which all atoms maintain the sp2 arrangement throughout. Different combinations of nanotubes (metallic and semiconducting) are considered. We further report IV characteristics of some of these junctions. This work was supported by NSF (ITR-022916), INTAS 00-237 and Russian program "Topics directed in condensed matter physics".

**KK0.18**

**Development of kinetic Monte Carlo simulator for initial nucleation process of nanoparticles.** Seichi Takami, Masao Umetu and Toshifumi Adachi, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Miyagi, Japan.

This study aims to develop a simulator that reveals the course of nucleation as well as the size- and shape-distribution of obtained nanoparticles. We developed a simulator that reveals the initial nucleation course of nanoparticles under given environmental conditions including pressure, temperature, and the concentration of source. This simulator is based on kinetic Monte Carlo method that facilitates connection between macroscopic parameters with atomic growth processes. In our simulator, the growth process of nanoparticles comprises three elementary processes, that is, sticking, diffusion, and desorption. The frequency of each process is calculated based on the environment conditions. In one simulation step, the simulator performs the following procedures. 1) Count all possible elementary processes and calculate their frequency. 2) Determine an elementary process to occur. 3) Change the shape of nanoparticle. To confirm the validity of our simulator, we studied the growth process of nanoparticles. Within the elapsed simulation time, the most seed particles stayed as vapor. However, once they grew larger than several Å, the size of nanoparticles continued to grow. This behavioral nucleation theory is an extended version of the classical nucleation theory. In this presentation, we will describe the results of simulation and comparison with classical nucleation theory.

**SESSION KK10**

**Other Systems**

Chair: Nicola Marani

Thursday Morning, December 4, 2013

Constitution A (70%)
Half-metallic ferromagnets, especially those which are compatible with III-V or II-VI semiconductors, are seen as a key ingredient in future high performance spintronic devices, because they have only one electronic spin channel at the Fermi energy and, therefore, may show nearly full spin polarization at quite high temperature. Although zinc-blend phases of MnSb and CrSb have been used as epitaxial nanodots or ultrathin films, it has not been possible to grow the zinclende half-metallic ferromagnetic phases in high-quality layers or films thick enough. However, spintronic devices require these films or layers. Therefore, theoretical exploration for these materials are highly desirable. We studied systematically all zinclende phases of transition-metal pnictides and chalogenides by using accurate full-potential density-functional method. We predicted the zinclende phases of MnBi and CrSb are excellent half-metallic ferromagnets. The half-metallic ferromagnetism of the zinclende CrSb phase is quite important because this phase has been fabricated. Furthermore, we proved that the zinclende phases of VTe, CrTe, and FeTe are the better half-metallic ferromagnets. They are not only low in energy with respect to the corresponding ground-state phases, but also mechanically stable against structural deformations, and therefore would be realized in the form of epitaxial films or layers thick enough for real applications. These half-metallic ferromagnetic phases should be useful in future spintronic applications because of their compatibility with the binary semiconductors. References: [1] Y-Q Xu, B-G Liu and D G Pettifor, Phys. Rev. B 66, 184435 (2002). [2] B-G Liu, Phys. Rev. B 67, 172411 (2003). [3] W-H Xie, Y-Q Xu, B-G Liu, and D G Pettifor, Phys Rev Lett, (accepted 2003).

10:15 AM EK10.6
Atomic Simulations of Impurity Effects in Grain Boundary Migration, Mikhail I Mendelev1, Seungwu Hye2 and David J Srolovitz3, MAE, Princeton University, Princeton, New Jersey; Princeton Materials Institute, Princeton University, Princeton, New Jersey.

The presence of impurities can alter the mobility of grain boundaries in a variety of ways. It is even more difficult to separate the effects of individual impurities on grain boundary migration through experiment since truly pure metals do not exist (ppm levels of impurities can greatly alter boundary properties) and because metals always contain a wide range of impurities. Therefore, experimental data on the impurity drag effect cannot be analyzed without the aid of supplementary atomistic computer simulation. In the present work, we studied the effects of Fe impurities on grain boundary motion in Al. The first step was to construct appropriate interatomic potentials. Potentials for pure Al and Fe were fitted to perfect crystal properties (lattice parameter, unrelaxed vacancy formation energy and elastic constants), interstitial formation energies and liquid density profiles in a liquid model obtained from the first principles calculations. These potentials provide good agreement with crystal and defect data, liquid diffusion data and melting points (the latter two were not included in the fits). The cross-potential for alloys were fitted to lattice parameters and formation energies of Al-Fe compounds and forces in a liquid configuration obtained from first principles calculations. The second step was to simulate the stress-driven motion of flat boundaries in pure Al using molecular dynamics (MD). Thirdly, we examined the effect of Fe impurity atoms on the same boundaries in Al. The segregation isotemps and the heats of segregation were determined using Monte Carlo simulations. Then the diffusivity of Fe in bulk Al and on the boundary was estimated using MD. Finally, we performed MD simulations of the motion of grain boundaries in Al containing several Fe atoms. The Fe atoms substantially slowed the boundary migration. The simulation results were compared with classical models of the impurity drag effect and the experimental data on grain boundary motion in Al.

10:50 AM EK10.7
Combining Ab-Initio Computations with Experiments for Designing High Energy-Density Electrode Materials for Advanced Lithium Batteries, Shirley Ying Meng1, Yin Wei Tan2, Bing Jue Huang1, Yi Li3,1 and Gerbrand Ceder3,1,2,3, Advanced Materials for Micro- & Nano- System Programme, Singapore-MIT Alliance, Singapore, Singapore; National University of Singapore, Singapore; National University of Singapore, Singapore; Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Density Functional Theory has been used successfully to predict and...
rationalize the properties of materials. The ability to do property
determination and optimization, while tremendously useful, leaves
materials synthesis, processing and optimization, as the bottleneck in
materials development. In an effort to shorten the design cycle of
advanced materials we have integrated ab initio computations with
experimental research in all phases of the development of electrodes
for rechargeable Li batteries. An initial search with Density
Functional Theory to sort through potential cathode materials based
on their Li intercalation potentials and electronic structure identified
certain Fe-containing compounds as good substitutes for current
battery materials. Crystal structure predictions and calculated mixing
enthalpies were used to guide the synthesis conditions and explain
experimental results. Motivated by the first principle calculation
results, LiNi4/3Fe2/3Co1/3Mn1/3O2 (LICMO) cathode materials
were synthesized by a sol-gel method. X-ray photoelectron
spectroscopy was used to confirm the electronic behavior predicted
with the first principles methods. This approach has produced
competitive electrode materials with very few iteration steps in the
design cycle. We believe that such direct integration of ab initio
methods with experimental research holds promise for significantly
shortening the development cycle of materials.

10:45 AM KK10.8
Molecular Dynamics Simulation for Structure and Dynamics
of Interstitials in Metals, Yoshihiko Kogure¹, Toshio Kosugi²,
Masao Doiyan³ and Hideo Kubozaki⁴, "Environmental Materials,
Tokyo University of Science & Technology, Ueno, Yamashita,
Japan; 5Japan Atomic Energy Research Institute, Tokai-mura,
Hirakata, Japan.

A large number of mechanical relaxation peaks have been observed in
the temperature dependence of high frequency ultrasonic attenuation
and internal friction in crystals. The defects 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 mechanics model developed by Novick et
al., in which the point defect strain per unit concentration is called as
"the elastic dipole". Recently, Granato has developed the
interstitial model (1992) and the model has successfully been
applied on thermal and mechanical phenomena of glass and liquid, in
which the dynamical character of the interstitials play essential role
as an elementary process. To investigate the fundamental mechanisms
of internal friction by interstitials in Cu and Al crystals, a molecular
dynamics simulation has been performed. Several potential functions
are adopted to express the atomic interaction. An embedded atom
method potential developed by present authors is also used in the
calculation. The atomic displacement and the elastic field around
the self or mixed interstitials in Cu and Al crystals are calculated
under the periodic or free boundary conditions. Then the relaxation
strength and the relaxation time for the interstitials are estimated.
The interaction between point defects through the strain field is also
important, that may cause a distribution of relaxation time and a
glass-like behavior. The effects of temperature on the structure and
the dynamics of point defects are also investigated by the simulation
under constant temperature conditions.