SYMPOSIUM EE

Linking Length Scales in the Mechanical Behavior of Materials

March 29 - 31, 2005

Chairs

T. J. Balk
Dept. of Chemical & Materials Engineering
University of Kentucky
177 F. Paul Anderson Tower
Lexington, KY 40506-0046
859-257-4582

Robert E. Rudd
Lawrence Livermore National Laboratory
L-045
7000 East Ave.
Livermore, CA 94550
925-422-4292

Noam Bernstein
Center for Computational Materials Science
Naval Research Laboratory
Code 6390
4555 Overlook Dr. SW
Washington, DC 20375
202-404-8628

Wolfgang Windl
Dept. of Materials Science & Engineering
Ohio State University
491 Watts Hall
2041 College Rd.
Columbus, OH 43210-1178
614-247-6900

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* Invited paper

SESSION EE1: Linking Atomistic and Continuum Length Scales
Chairs: Noam Bernstein and Mark Robbins
Tuesday Morning, March 29, 2005
Room 2018 (Moscone West)

8:30 AM *EE1.1
Multiscale Simulations of Materials: From Covalent to Metallic Solids, Tests and Applications. Efthimios Kaxiras, [1]Physics, Harvard University, Cambridge, Massachusetts; [2]Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts.

A range of physical phenomena require the description of a solid at several scales simultaneously. Some characteristic examples are corrosion and embrittlment of metal alloys, brittle and ductile fracture, especially as they are influenced by chemical impurities. The successful application of multiscale methods requires seamless coupling of the regions where different methodologies are employed, from the atomistic quantum mechanical region, to the classical atomistic, to the elastic continuum. Of equal importance is the use of efficient and accurate methodologies, especially in the atomistic regions. In this talk I will review recent progress in developing multiscale simulations for materials and especially for metallic solids, where the atributes of accuracy and efficiency of the methodology are often in conflict. I will present results from tests and on-going applications of these methods, and will provide an evaluation of the prospects for realistic, multiscale simulations for systems of practical interest.

9:00 AM EE1.2
Structure of Dislocations in FCC Metals as a Function of Temperature using the Quasicontinuum Method.
Laurent Dupuy[1], Ellad Tadmor[2], Ron Miller[3] and Rob Phillips[4]; [1]Lawrence Livermore National Laboratory, Livermore, California; [2]Technion - Israel Institute of Technology, Haifa, Israel; [3]Carleton University, Ottawa, Ontario, Canada; [4]California Institute of Technology, Pasadena, California.

The quasicontinuum method is a mixed continuum and atomistic approach for simulating the mechanical response of polycrystalline materials. It allows large-scale atomistic calculations to be performed on moderately small computers. This method was recently extended to study the behavior of defects at finite temperature. The principle of this method is briefly recalled. Its applicability and its limitations are discussed. As an example, the structure of dislocations, in particular the splitting distance between the two partial dislocations, is discussed as a function of temperature for three different FCC metals. The results are compared to full atomistic calculations. Acknowledgement: This work was performed in part under the auspices of the US Dept. of Energy at the University of California/Lawrence Livermore National Laboratory.

9:15 AM EE1.3
Integrated Green's Function/Molecular Dynamics Method for Linking Length Scales in Modeling of Nanostructures.
Vinod K. Tewary and David T. Read; Materials Reliability, National Institute of Standards & Technology, Boulder, Colorado.

A method is described for multiscale modeling of the mechanical behavior of nanostructures embedded in solids containing a free surface. The method links seamlessly the length scales from atomistic to macro in an integrated formalism. It is based upon the use of lattice-statics and continuum Green's functions integrated with molecular dynamics. A modified form of molecular dynamics is used to calculate the equilibrium configuration of atoms in and close to the nanostructure; these atoms are coupled to the host lattice through the lattice statics Green's function. This gives a fully atomistic description of a nanostructure that includes the effect of nonlinear forces, embedded in a large crystallite consisting of a million atoms or more. The lattice statics Green's function is then related to the anisotropic continuum Green's function that is used to model the free surface and the far field. Thus the method fully accounts for the nonlinear discrete lattice effects inside and close to the nanostructures, linear response of the discrete lattice at the atomistic scale near the nanostructure and the macroscopic continuum behavior of extended defects such as a free surface, interfaces, and dislocations. The method relates the discrete lattice distortion at the atomistic scales to measurable parameters of mechanical properties at macro scales such as the displacement and strain fields at the free surface without any need for arbitrary averaging algorithms. A major advantage of the lattice-statics Green's function is that it can model a large crystallite containing a million atoms or more without excessive CPU effort. The method consists of writing the response of a solid in terms of lattice-statics Green's function and the Kanzaki force that accounts for discrete structure of the lattice as well as local nonlinear effects. The lattice-statics Green's function is calculated by using the discrete Fourier transform technique. The Kanzaki force is calculated by using molecular dynamics. The calculation proceeds by a coupled iteration that alternates between molecular dynamics and Green's function relaxations. Numerical results will be presented for the stress and strain fields due to a gold nanoinclusion in copper and a germanium quantum dot in silicon containing free surfaces.

9:30 AM EE1.4
Local Stresses and Elastic Constants and the Link to the Continuum. Terry J. Delph, Dept. of Mechanical Engineering & Mechancis, Lehigh University, Bethlehem, Pennsylvania.

We report here on some recent investigations regarding local stresses and elastic constants at the atomic scale and their relationship to the corresponding continuum level quantities. As is the case on the continuum level, one may define two different stress measures at the atomic scale: the local second Piola-Kirchoff (PK2) stress and the local Cauchy stress. The widely used atomic stress turns out to be a particular case of the former. The latter has attracted considerable recent attention in atomistic calculations. We give general expressions for both of these and demonstrate that expressions for the local Cauchy stress may be derived for quite general multibody potentials. Examples using the three-body Stillinger-Weber potential for silicon are presented. We likewise discuss how atomistic level expressions for the local elastic constants may be derived, even in situations in which the underlying atomic structure lacks periodicity. Finally, we focus upon a simple integral averaging technique that yields computable expressions for both the local stresses and the local elastic constants. We demonstrate that these integral averages smoothly approach their continuum level counterparts as the averaging volume becomes large.

9:45 AM EE1.5
Explicit Dynamics in Quasicontinuum Method.
Benjamin L. Hansen[1], Jaime Marian[2,1], Jaroslaw Knap[1] and Michael Ortiz[1]; [1]California Institute of Technology, Pasadena, California; [2]Lawrence Livermore National Laboratory, Livermore, California.

The Quasicontinuum (QC) model is a method for coarse-graining lattice systems in a seamless way by using appropriate kinematic constraints, summation rules and resolution adaption. In its original formulation, QC is a quasistatic method that contains lattice statics and continuum elasticity as limit cases. However, dynamic phenomena of interest in many physical processes, such as thermally activated defect motion, are not captured in the present form. Here, we propose a generalized QC method that incorporates Brownian (Langevin) dynamics and accounts for lattice vibrations in the coarse system. The equations of motion at the nodal level are integrated by way of an explicit Newmark algorithm. As a preliminary evaluation the thermal expansion coefficient, α of Al is performed at several temperatures. Simulations are first carried out for the purely atomistic limit case. As well, computations of α are performed for coarse samples in which the sensitivity of this parameter to several QC-implementation variables is studied.

10:30 AM *EE1.6
A Hybrid Atomistic/Continuum Method Applied to Fluid Flow and Solid Contact. Mark O. Robbins[1,2], Noam Bernstein[4], Shiyi Chen[2], Judith Harrison[3], Sangil Hyun[1,2], Jin Liu[2], Binquan Luan[1], Jean-Francois Molinari[2] and Xiaobo Nie[1,2]; [1]Physics and Astronomy, Johns Hopkins Univ., Baltimore, Maryland; [2]Mechanical Engineering, Johns Hopkins University, Baltimore, Maryland; [3]Chemistry, United States Naval Academy, Annapolis, Maryland; [4]Center for Computational Materials Science, Naval Research Laboratory, Washington, District of Columbia.

A general approach will be presented that describes most regions of space with continuum methods, but treats interfacial and high stress regions with classical molecular dynamics [1]. Both atomistic and continuum approaches are used in an overlap region, and provide boundary conditions for each other at the edges of this region. For fluids the boundary conditions are expressed as particle fluxes, while for solids atomistic displacements are used. Applications to three intrinsically mutiscale problems will be described. The first is flow in a cavity driven by a moving wall [1]. Continuum mechanics with a no-slip boundary condition predicts a diverging stress at the corner where moving and static walls meet, and an infinite force on the moving wall. This singularity is resolved by using atomistic simulations in the corner and cavities with mm dimensions are treated. The separation between the intrinsic time scales of the continuum and atomistic regions is spanned for steady-state flow, leading to a total speed up by more than 10 orders of magnitude compared to an all atomistic treatment. The second problem is the motion of an interface between two fluids over a solid. This leads to similar singular stresses, and has the additional complication of a flexible fluid interface. The final example is contact between rough surfaces. Here atomistic interactions at surfaces dominate adhesive interactions and friction, while the contact geometry depends on elastic deformations at large scales. The hybrid approach is used to

determine the scaling of friction and adhesion with system size for self-affine surfaces. 1. X. B. Nie, S. Y. Chen, W. N. E, and M. O. Robbins, J. Fluid Mech. 500, 55 (2004). X.~B. Nie, S.~Y. Chen, and M.~O. Robbins, Phys. Fluids 16, 3579, (2004).

11:00 AM EE1.7
Quasicontinuum Study of Multiple Void Interaction/Void Coalescence in Al. Jaime Marian[1,2], Jaroslaw Knap[2] and Michael Ortiz[2]; [1]Chemistry and Materials Science Directorate, Lawrence Livermore National Laboratory, Livermore, California; [2]Division of Engineering and Applied Science, California Institute of Technology, Pasadena, California.

Void nucleation, growth and coalescence are known to be part of a sequence of events leading to dynamic ductile fracture in metals. These processes require the outbreak of plastic flow in order to transport matter to and from the voids resulting in the formation of larger cavities and microcracks. Although having consequences of macroscopic importance, void growth and coalescence are phenomena essentially atomistic in scope and, thus, experimental techniques can provide only limited information about the pertinent mechanisms. However, plastic flow, although very localized, involves long range stress fields associated to dislocations and its study requires the use of appropriate boundary conditions that will not incur in undesirable numerical artifacts or unrealistic behavior. Therefore, molecular dynamics and statics methods are insufficient to treat the full scope of the problem and complementary calculations are required. In this work we use the Quasicontinuum (QC) method to study the processes of void growth and coalescence in Al. QC is a method for coarsening lattice systems by using a set of kinematic constraints coupled with special lattice summation rules and mesh adaptivity. Therefore, QC provides a seamless coupling across the scales and contains lattice statics and continuum elasticity as limit cases. Results for single void growth under different loading conditions and two-void interactions are presented.

11:15 AM EE1.8
Atomic Scale and Continuum Simulations of Island Coalescence During Thin Film Growth. Edmund B. Webb[1], Steven C. Seel[1] and Jonathan A. Zimmerman[2]; [1]Sandia National Laboratories, Albuquerque, New Mexico; [2]Sandia National Laboratories, Livermore, California.

Given the significant presence of thin film technology in a wide array of applications, a thorough understanding of microstructure/property relations is highly desirable. To this end it is important to be able to describe stress evolution during thin film growth since residual stresses can influence subsequent microstructure evolution as well as mechanical response. This problem is inherently multiscale. Atomic scale detail is important, particularly for elucidating relaxation mechanisms at various stages of film growth (isolated islands, island coalescence). However, it is also clear that continuum descriptions are sufficient at some scale and far more computationally efficient. A natural problem emerges in understanding in what situations atomic scale detail is beneficial or, perhaps, necessary. We present results from a study combining atomic simulations with finite element calculations to explore stress evolution during thin film growth. Our focus is on island coalescence that occurs when isolated islands grow and eventually impinge on one another during, for instance, Volmer-Weber growth. Molecular dynamics (MD) and Monte Carlo (MC) methods have been used to examine coalescence for island sizes from D = 2 - 200 nm in a parallel hemi-cylindrical capping geometry, where D is the cylinder diameter. Atomic interactions are governed via embedded atom method potentials and the zero mismatch case of Au islands on Au(100) is modeled. While it is expected that the elastic process of coalescence can be captured on MD time scales, this is verified for a few cases by comparing equilibrated MD structures to those obtained from MC calculations. Coalescence height h is calculated and demonstrated to behave in accord with continuum predictions for large islands but, for the smallest sizes studied, deviations from this behavior were observed. This is shown to coincide with an onset of more significant atomic relaxations which are, in turn, related to very high stress states prior to relaxation and coalescence. A challenge for atomic scale simulations is to quantitatively predict stress in structures containing interfaces or free surfaces. This is overcome using a spatial homogenization technique that permits more robust estimates of stress in very small volume elements near surfaces. With this, calculated stress distributions in pre-coalescence and coalesced structures are presented to further elucidate the cause of observed relaxations. These distributions are also shown to be useful when evaluating the need for atomic scale detail as compared to that provided by continuum simulations. Closing discussion will review initial results in studying the case of Ni islands on Au(100).

11:30 AM EE1.9
Modelling the Nanoindentation Test using Molecular Dynamics, Dislocation Dynamics and Continuum Mechanics. Marc C. Fivel[1], Marc Verdier[2], Ludovic Charleux[1,2] and David Rodney[1]; [1]CNRS/INPG, GPM2, St Martin d'Heres, France; [2]CNRS/INPG, LTPCM, St Martin d'Heres, France.

In this study, molecular dynamics (MD) are used to derive a criterion for the dislocation nucleation in pure fcc crystals (Ni). The indenter is taken as a pure sphere represented by a repulsive potential. Indentations of (111) single crystal of Ni are simulated for several sizes of the sphere and simulation box and both in lattice static (T=0K) and in molecular dynamics (T=300K) modes. It is found that the onset of plasticity occurs below the surface as predicted by elastic models. Then, a complex dislocation structure quickly develops and prismatic loops are generated through a process involving cross-slip. The shape and position of the prismatic loops are explicitly given by the MD simulations. This defines a nucleation criterion for dislocation dynamics (DD) simulations which are performed at the higher scale. In these simulations, both the dislocation microstructure and the actual shape of the indented surface are computed and updated during the indentation process. This gives access to the real contact area between the indenter and the material and consequently to the exact hardness of the material. These results from DD simulations are finally compared to different models of continuum mechanics. Special attention is paid to the indent size effect.

11:45 AM EE1.10
An Atomistic-Based Quasicontinuum Method.
Chuin-Shan Chen, Chang-Wei Huang, Ying-Pao Liao and Jia-Wei Lai; Department of Civil Engineering, National Taiwan University, Taipei, Taiwan.

We present a novel quasicontinuum method from an atomistic perspective. A coherent formulation for accurate energy and force calculations is developed through careful padding of kinematically constrained atoms. An atomistic-based error estimator based only on the current lattice configuration is developed for adaptive selection of representative atoms. Application of the method is extended to three dimensions in which the representative atoms are triangulated with a set of tetrahedra using an efficient Delaunay-based mesh generator. An adaptively remeshing strategy controlled by an error density function is developed. Verification examples are designed to demonstrate accuracy and efficiency of the proposed method. In addition, the method is used to study deformation processes of nanowire indentation and numerical results are compared with in-house experimental measurements.

SESSION EE2: Linking Scales in Fracture and Friction
Chairs: Mukul Kumar and Robert Rudd
Tuesday Afternoon, March 29, 2005
Room 2018 (Moscone West)

1:30 PM *EE2.1
Investigating The Instability Dynamics Of Brittle Fracture By Computer Simulation. Farid Abraham, [1]LLNL, Livermore, California; [2]University of Georgia, Athens, Georgia.

One of our most intriguing findings is a dynamic instability of the crack tip in rapid brittle fracture that prevents a crack from achieving its theoretical steady-state speed equal to the Rayleigh wave speed. Continuum fracture theory typically assumes that cracks are smooth and predicts that they accelerate to a limiting velocity equal to the Rayleigh speed. In contrast, experiment tells us that, in a common fracture sequence, an initially smooth and mirror like fracture surface begins to appear misty and then evolves into a rough, hackle region with a limiting velocity significantly below the Rayleigh speed. All of these features are unexplained using conventional continuum theory. Our atomistic simulations duplicate these experimental features and yield physical explanations for the dynamic crack instability. The Yoffe linear theory of dynamic brittle fracture suggests that crack motion will be unstable beyond ~70% of the Rayleigh speed, a prediction that is not supported by experiment. We show that hyperelasticity, the elasticity of large strains, plays a governing role in the instability dynamics of brittle fracture. A simple scaling model based on an effective elastic modulus, coupled with the Yoffe solution, gives successful predictions for the onset speed of the crack instability.

2:00 PM EE2.2
Influence of Ni Additions on the Deformation Mechanisms at Crack Tips in Ferrite. Michael J. Luton[2], Peter A. Gordon[2], Ruohua Z. Guo[2] and Diana Farkas[1]; [1]Materials Science, Virginia Tech, Blacksburg, Virginia; [2]Corporate Strategic Research, ExxonMobil Research & Engineering Co, Clinton Township, New Jersey.

Model empirical interatomic potentials are used to study deformation

mechanisms at crack tips in bcc Fe containing substitutional Ni additions. Molecular statics techniques are used to simulate the atomic level configuration of the crack tip region for various crack orientations with and without Ni additions. The deformation mechanisms observed at the crack tip are governed by the emission of lattice dislocations from the crack tip. Twinning is also observed as an alternative deformation mechanism. It is found that Ni additions result in increased ease of dislocation emission from the crack tip. These results can be rationalized in terms of the effect of Ni on the unstable stacking fault energy and the surface energy. Ni additions result in increased ductility and crack tip blunting, as well as a decreased tendency for twinning as a crack tip deformation mechanism.

2:15 PM EE2.3
Influence of Microstructural Length Scales on Dynamic Failure. Mukul Kumar, Roger Minich and James Stolken; Lawrence Livermore National Laboratory, Livermore, California.

The scaling of mechanical properties with microstructural length scales, such as grain size, is well known. In addition, the role that grain boundary networks play during failure processes such as stress corrosion cracking, creep cavitation, and weld cracking has also been well documented for metallic materials. These processes have been characterized both at the microscopic and mesoscopic scale, though the role of grain boundary crystallography is only recently starting to emerge. For instance, it has been shown recently that the Hall-Petch scaling of yield stress with grain size needs to be reformulated to take into account a parameter called grain boundary character distribution that is related to the frequency of so-called special boundaries in the microstructure. Less well developed is an understanding of the role of microstructures in the process of void nucleation and growth leading to failure during shock loading of materials. In this paper, we shall report on the scaling recently observed in the case of dynamic failure or spall under shock deformation conditions for different microstructures in high purity copper. The spall strength is observed to increase as the length scales coarsen, which is counter to the Hall-Petch relationship, eventually leveling off for single crystals. The role of nucleation site density and grain boundary character distribution in understanding this behavior as a function of impact pressure will be explored in the context of the scaling laws that emerge from this data. This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

2:30 PM EE2.4
Quantum-Mechanically-Informed Kinetic Monte Carlo Simulations of Void Nucleation Under Spall by Vacancy Diffusion and Clustering. Santiago A. Serebrinsky[1], Michael Ortiz[1], Mitchell Ong[2], Kyle Caspersen[2], Gregory Ho[2] and Emily A. Carter[2]; [1]Graduate Aeronautical Laboratories, California Institute of Technology, Pasadena, California; [2]Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey.

Spallation failure is observed in many materials. A common observation is the formation of small voids surrounded by severe plastic deformation. Detailed mechanistic understanding of the sequence of processes underlying such behavior is lacking as yet. In this work, we analyze the feasibility of vacancy diffusion and clustering as an operative mechanism during the early stages of spallation in aluminum. The role envisioned for the vacancy mechanism is that of nucleating nanometer-sized voids that can later cavitate by plastic deformation. The method applied involves a combination of first principles density functional theory and lattice gas kinetic Monte Carlo (KMC) calculations. Density-functional theory calculations are used to determine the effect of pressure on the activation energy barrier Ea for vacancy migration. It is found that Ea decreased by approximately 25% at a tensile hydrostatic stress of 7GPa. These first principles results are used to inform KMC calculations of vacancy diffusion in an Al lattice. The simulations predict high nanovoid nucleation rates, especially in the vicinity of grain boundaries.

2:45 PM EE2.5
On the Role of Multi-Length-Scale Microstructural Correlations in the Fracture of Grain Boundary Engineered Materials. Bryan Reed, Eira T. Seppala, Mukul Kumar, Roger W. Minich and Robert E. Rudd; Lawrence Livermore Natl. Lab, Livermore, California.

We report on a combined theoretical/experimental project to explore the role of crystallographic correlations on the roughness scaling properties of intergranular fracture surfaces. The focus is on grain boundary engineered (GBE) materials, which are processed to optimize the fraction of strong or "special" boundaries taking part in the grain boundary network in an essential way. Requirements of crystallographic consistency dictate certain correlations in the grain boundary networks of these materials, which in turn alter the fracture properties. The role of "short-range" (i.e. acting on a single triple junction at a time) correlations in altering the percolation behavior is fairly well understood, but a group-theoretical analysis suggests that similar correlations may be acting on all distance scales. The magnitude and role of these additional correlations is only now being investigated. On the computational side, we developed a method of efficiently generating microstructures that account for all of the constraints underlying these correlations and which may be tuned to reproduce the statistics in a specific GBE material. These microstructures are computationally "fractured," yielding a theoretical prediction of the roughness scaling exponents. Experimentally, we have measured the roughness of GBE and non-GBE fracture surfaces and discerned some very significant differences. Under identical fracture conditions the Hurst exponents are much larger ($\sim$0.8 compared to $\sim$0.6) in the non-GBE material, suggesting significantly different mechanisms in the two cases; the non-GBE exponents also appear to be less isotropic and less uniform. We will interpret these trends in light of the computational results and discuss possible implications for the reliability of GBE versus non-GBE materials. This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

3:30 PM *EE2.6
Multi-Length Scale Experiments and Modeling of Friction: Connecting Micro-Device Performance with Nano-Scale Contact Behavior. Robert W. Carpick[1], Erin E. Flater[1], Can K. Bora[1], Michael E. Plesha[1], Anirudha V. Sumant[1], Mark D. Street[1], Maarten P. de Boer[2], Alex D. Corwin[2] and E. David Reedy[2]; [1]Engineering Physics, University of Wisconsin - Madison, Madison, Wisconsin; [2]Sandia National Laboratories, Albuquerque, Wisconsin.

The emergence of nano-scale materials and devices has highlighted the need to control surface and interface properties due to the divergence of the surface-to-volume ratio as the number of atoms is reduced to the atomic limit. In particular, friction, adhesion, and wear are critical factors in micro- and nanomechanical devices, and they are yet to be well-understood or controlled. We use atomic force microscopy (AFM) to resolve multi-scale roughness of silicon-based micromachine surfaces, and to determine the tribological behavior of nano-scale single asperity contacts. We study self-assembled monolayer (SAM) coatings applied to both the sample and the AFM tip, so that the experiment properly represent the asperity size, shape, and composition found in actual devices. Our work is compared with joint studies at Sandia National Laboratories using a MEMS device designed for quantitative friction and wear tests. We show that the nanoscale (AFM) and microscale (MEMS) friction behavior of these interfaces correlate closely. In particular, an increase in friction with fluorination of the monolayer is observed and quantitatively evaluated using an adhesive contact mechanics model that has been modified to account for the SAMs' mechanical properties. As well, microscale measurements in the MEMS test device indicate that a long chain molecule SAM exhibits viscous behavior, while short chain molecules do not. We describe AFM experiments tailored to examine the nanoscale origins of this effect. Finally, we present results aimed at determining the structural and chemical effects of wear in the device by using high resolution synchrotron-based chemical imaging. In partcicular, we show using photoemission electron microscopy (PEEM) that removal and modification of SAM molecules occurs during the sliding process in the actual device. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the US Department of Energy under contract DE-AC04-94AL85000.

4:00 PM EE2.7
Concurrent Multiscale Modeling of Contact and Friction with Multiple Asperities. Frederic Sansoz[1] and Ron Miller[2]; [1]Department of Mechanical Engineering, University of Vermont, Burlington, Vermont; [2]Department of Mechanical and Aerospace Engineering, Carleton University, Ottawa, Ontario, Canada.

The mechanics of contact and friction between nanoscale asperities has drawn a considerable interest in recent years because of its importance to MEMS tribology, nanoindentation, scanning probe microscopy, and coating deformation. Despite common knowledge that the surface of a thin film is not atomically flat, the influence of multiple surface asperities on contact/friction mechanics is not fully understood. For example, it is unclear how the presence of nanoscale asperities, which creates highly-stressed points of contact, significantly alters the incipient plasticity of indented or scratched films. In this study, we measure at various length scales the topography of electrodeposited metal surfaces using atomic force microscopy. The indentation and tribology of those rough surfaces are investigated by multiscale atomistic simulations using the quasicontinuum theory. The model consists in the contact and friction of a single asperity on a rough FCC crystal surface containing multiple nanoscale asperities. Special emphasis is placed in the analysis of asperities deformation in

relation to the plastic behavior of the film surface.

4:15 PM EE2.8
The Length Scale for Dynamic Spallation Fracture in Crystalline Metals. James Belak, John Kinney, Mukul Kumar and Roger Minich; Physics, University of California, Lawrence Livermore National Laboratory, Livermore, California.

We present experimental results for the length scale for void growth during dynamic spallation fracture in single crystal aluminum and vanadium. Shock-induced spallation fracture in ductile metals is an internal rupture process in which voids nucleate, grow and link to from a fracture. Using soft-recovered incipiently spalled samples, we measured the 3D distribution of voids with synchrotron-based x-ray tomography. The void size distribution is bimodal with small and large voids. The mean spacing of large voids is determined from the competition between the high strain rate loading and the rate of release of elastic energy as the voids grow. Work performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

4:30 PM EE2.9
Bridging Length Scales in Models for Crack Predictions in Hardening Concrete Structures. Eddy Koenders[1] and Klaas van Breugel[2]; [1]Design and Construction, Delft University of Technology, Delft, Netherlands; [2]Micromechanical Laboratory, Delft University of Technology, Delft, Netherlands.

The production of a sustainable high quality building material like concrete, is demanding for a clear and fundamental understanding of all its (internal) properties. Depending on the level of observation, different constituents are involved and implicitly determine the modelling approach. From this, the multi-scale modelling approach has been born comprising three levels of observation, viz. macro, meso and micro level. With respect to simulation of the material properties that associate with these particular levels, emphasis is on the level on which these models run. In order to make these models compatible, these different length-scales have to be bridged. For concrete in particular, simulation models are available for predicting different kinds of material properties. Models used for simulation of the microstructural development, are expressed in terms of the degree of hydration. The output results of these hydration models are used as input for stress-calculation models, which predict the concretes sensitivity towards thermal cracking. Whereas the hydration models run internally on a nano- to micro-length scale, the stress-calculation models run on a meso- to macro-scale level, introducing a length-scale gap. With the increasing trend of fundamental material research towards a more detailed molecular level, this length-scale gap will even become larger. In this contribution, both the hydration model and the stress-calculation model will be presented, with emphasis on the internal length-scales on which they run. It will be discussed how in-depth microstructural modelling contributes to the reliability of crack predictions for macro-scale concrete elements. The inclusion of the scatter of micro-scale parameters, and with this, the consequences for the larger-scale stress calculations will be discussed in terms of a probabilistic approach. This provides a more profound basis for the Monte Carlo approach, which include the parameter variations that act at the broad range of length scales. The paper ends with conclusions.

4:45 PM EE2.10
The Effect of Particle Size on Fracture Properties and Size Effect of Concrete. Erik Schlangen[1], Heng Soon Lim[1] and Jaap Weerheijm[1,2]; [1]CiTG, Microlab, Delft University of Technology, Delft, Netherlands; [2]TNO-PML, Rijswijk, Netherlands.

Structural behaviour of concrete structures is often tested on laboratory test. For this purpose the size of the structure is scaled down with a factor of about 3 to 10. To obtain accurate results also the material has to be scaled in the material used for preparing the specimens that are tested. This implies using smaller aggregates, which influences of course the mechanical behaviour of the material. Although this is an important effect, it is not known how large this influence of scaling of the material structure is on the fracture behaviour of concrete. Furthermore it is known that a strong size effect exists in concrete fracture strength, which complicates the interpretation of laboratory scaled tests even further. In the study the effect of scaling the material structure on the fracture behaviour of concrete is investigated. Next to this the size effect of concrete fracture strength and fracture energy is studied. In the paper a description is given of the research, which is a combination of numerical modelling and experiments. The fracture mechanism of concrete made with different size aggregates are tested experimentally. Numerically a lattice type fracture model [1, 2] is adopted to simulate the fracture mechanisms in concrete. The heterogeneity of the concrete is implemented in different ways. Simulations on various scales, ranging from micro- to macroscale are performed. The results obtained show a clear relation between the size of spherical particles in the concrete and the width of fracture process zone and fracture energy. The scale effect of concrete can be partly explained by this relationship. [1] Schlangen, E. and Garboczi, E.J., Fracture simulations of concrete using lattice models: computational aspects, Engineering Fracture Mechanics, 57(2/3): 319-332, 1997. [2] Schlangen, E., Koenders, E.A.B. and van Breugel, K., Formation of eigenstress and cracks due to autogenous shrinkage. In Li V. C., Leung C. K. Y., Willam K. J. and Billington S. L. (eds.), Fracture Mechanics of Concrete Structures, pp. 447-454, 2004.

SESSION EE3: Poster Session: Bridging Length Scales for Surfaces and Interfaces
Chairs: John Balk, Noam Bernstein, Robert Rudd and Wolfgang Windl
Tuesday Evening, March 29, 2005
8:00 PM
Salons 8-15 (Marriott)

EE3.1
Roughness Exponents, Microstructure, Correlation Length, and the Quantum Origin of Self-Affine Fracture.
Moises Hinojosa, Jorge Aldaco, Raul Rodriguez and Ubaldo Ortiz; Div. de Ingenieria Mecanica, FIME-UANL, San Nicolas de los Garza, Nuevo Leon, Mexico.

The self-affine character of the fracture surfaces of metals, polymers, ceramics and composites has been well documented over the past two decades. It has been established that the fracure surfaces and rupture lines are self-affine objects characterized by so called 'universal' roughness exponents independent of the microstructure and the loading conditions. Here we show that the self-affine correlation length is closely associated with the microstructure heterogeneities. We also explore the possibility of the existence of attractor values that govern the fracture process, as opposed to universal exponents. The quantum origin of this behavior is also discussed in terms of the density functional theory-exact universal exchange-correlation potential.

EE3.2
Surface Roughening of Metal-Polymer Interfaces during Uniaxial Plastic Deformation. R. van Tijum[1,2,3], W. P. Vellinga[1,2,3] and J. Th. M. DeHosson[1,2,3]; [1]Applied Physics, University of Groningen, Groningen, Netherlands; [2]Materials Science Centre, Groningen, Netherlands; [3]Netherlands Institute for Metals Research, Delft, Netherlands.

In an increasing number of applications metal-polymer laminates are produced as plates and afterwards formed to their final shape. During forming large deformations occur that result in roughening of the polymer surface affecting the mechanical integrity of the system. In this paper we present a numerical study focusing on the influence of roughening of the metal substrate on the final roughness of the polymer outer surface. The metal-polymer system is loaded under uniaxial tension. The polymer coating is described by various stages of deformations that mimic the response of Poly Ethylene Terephthalate. For the interface between the metal and the polymer a mixed-mode cohesive zone is used characterized by adhesive energy, working distance, maximum stress and a normal/shear ratio. The substrate is a self-affine rough rigid material as characterized by the so-called Hurst exponent, the correlation length and the RMS roughness. These parameters as a function of strain were taken from experiments. Up to yielding we find that the polymer surface is smoother for thicker coatings. It implies that the RMS roughness is lower, the Hurst exponent is higher and that the correlation length at the outer surface becomes higher than the values at the interface between the polymer coating and the substrate. Above the yield point of the polymer, the macroscopic stresses reduce, causing likewise an easier transfer of the roughness of the interface through the polymer coating. This results in a rougher outer surface of the polymer coating. For coatings much thicker than the correlation length of the rough interface this results in a higher RMS roughness than the interface. In the hardening phase of the polymer coating, the RMS roughness is reduced.

EE3.3
Abstract Withdrawn

EE3.4
Interaction between Cracking, Delamination and Buckling in Elastic Brittle Thin Films. W. P. Vellinga[1,2], J. Th. M. De Hosson[1] and M. G. D. Geers[2]; [1]Materials Science, Applied Physics, University of Groningen, Groningen; [2]Materials Technology, Mechanical Engineering, Eindhoven University of Technology, Eindhoven, Netherlands.

A mesoscopic model that describes the interaction of cracking,

delamination and buckling in the deformation of brittle, disordered, elastic coatings is presented. The model consists of three layers of linear springs, representing substrate, interface and coating. Springs in the interface and the coating can break. Both breaking strain and geometry may be used to mimic disorder in the coating and interface. The thickness of the coating is incorporated in a way that leads to realistic bending behavior. It is shown that the model reproduces experimental results in which cracking, delamination and buckling interact in a qualitatively correct way; more specifically: in uniaxial tension of films with an internal compressive stress, the initiation of buckles above delaminated areas near crack edges in the model is very similar to the phenomena found in experiments. The key role of the stress transfer correlation length in the scaling behavior of 2D brittle fracture of thin films is investigated for all relevant geometrical and material properties. Deviations from this regime are shown to occur when propagation, disorder and/or delamination play a role. Applications of the model to crack propagation along disordered interfaces will be shown.

EE3.5
Transferred to EE7.4

EE3.6
Atomistic Simulation of Growth of Amorphous C:H Films. Matous Mrovec and Christian Elsaesser; Fraunhofer-Institut fuer Werkstoffmechanik, Freiburg, Germany.

Diamond-like amorphous C:H films have a number of outstanding properties for technological applications: For instance they are useful as hard and tough protective surface coatings of metals, or they serve as solid-state lubricants for low friction of fast rotating or sliding machine parts. Such films are grown by atomic or molecular vapor deposition. The experimental optimisation and control of deposition parameters for the production of high-performance films is a difficult technological task. Atomic-level understanding of the growth process and the resulting film structure can give valuable insights into process-property relations. This contribution reports a molecular-dynamics simulation study of amorphous a-C:H films grown by deposition of various hydrocarbon molecules. The interatomic interactions in real space were modelled by recently developed analytic bond-order potentials (ABOP) [1]. These ABOP were derived from tight-binding electronic-structure theory, and they describe different covalent bonds in molecular and crystalline environments with high transferability. Local structure and bonding properties of the films resulting from variations of some process parameters will be presented. [1] D. G. Pettifor, I. I. Oleinik, Phys. Rev. B 59 (1999) 8487, 8500.

EE3.7
Erosion of Graphite Surfaces by Energetic Ions in a Fusion Chamber: Coupling Molecular Dynamics and Continuum Plasma Simulations. Jaime Marian[1], Luis A. Zepeda-Ruiz[1], Eduardo Bringa[1], George H. Gilmer[1] and Thomas Rognlien[2]; [1]Chemistry and Materials Science Directorate, Lawrence Livermore National Laboratory, Livermore, California; [2]Physics and Advanced Technologies, Lawrence Livermore National Laboratory, Livermore, California.

Impurities arising from the surface layer of the graphite first wall due to the continued interaction with the plasma play a very significant role in the power balance of magnetic fusion reactors. A detailed model that accurately accounts for all the energy losses in the plasma due to wall interactions must include three distinct regions, each operating at a different space/time scale and each with its intrinsic mechanisms: i) the first wall material with emphasis on the thin surface, ii) the intermediate region of mixing between wall impurities and plasma, and , iii), the full plasma region. These regions involve processes of physical, mechanical and chemical nature and their interplay across the scales constitutes a characteristic multiscale/multiphysics problem. In this work we focus on molecular dynamics calculations of the sputtering yield of amorphous graphite layers as a function of variables that are output from chemical and plasma physics codes. The computed sputtering yield is fed back into continuum thermodynamics plasma in what has become a cross-informed self-consistent effort. Emphasis on the connections of the results presented here with the models pertinent to regions (ii) and (iii) is made.

EE3.8
Mass Transport via Cross-Slip of Screw Dislocations in FCC Metals. Yury Osetskiy[1], Roger E. Stoller[2] and Steven Zinkle[2]; [1]Computer Sciences and Math, ORNL, Oak Ridge, Tennessee; [2]Metals and Ceramics, ORNL, Oak Ridge, Tennessee.

Cross-slip is an important mechanism of dynamics of screw dislocations and interaction with obstacles to their glide and it also can serve as a powerful mechanism of mass-transport at nanoscale. In this paper we present example of nanoscale mass transport observed in atomic-scale dislocation dynamics studied by large-scale atomic-level modeling. We have considered gliding screw dislocations interacting with stacking fault tetrahedra (SFTs) of size of up to 12nm over the temperature range from 0 to 600K and microscopic strain rate from 5x106 to 108s-1 in copper. Two qualitatively different cases i.e. bulk metal and thin film with free surfaces, were simulated. It is demonstrated that a significant mass transport occurs during a screw dislocation-SFT interaction and the result depends on SFT size, temperature and strain rate. In the case of bulk dislocations mass transport occurs at relatively short distance splitting an SFT into parts separated up to few tens nm. In the case thin films a significant transport of vacancies to the surface was observed. The results obtained can be used in interpretation of experimental observations in irradiated and in-situ strained metals.

SESSION EE4: Dislocation Behavior; Multiscale Modeling and Characterization
Chairs: Dierk Raabe and Robert Rudd
Wednesday Morning, March 30, 2005
Room 2018 (Moscone West)

8:30 AM EE4.1
Constitutive Description of Dislocations, Gradients, and Grain Boundaries in Crystal Plasticity FEM. A. Ma, F. Roters and Dierk Raabe; Microstructure Physics, Max-Planck-Institut, Duesseldorf, Germany.

Crystallographic slip, e.g. movement of dislocations on distinct slip planes is the main source of plastic deformation in most metals. The crystal plasticity FEM combines this basic process with the Finite Element Method by assuming that the plastic velocity gradient is composed out of the shear contributions of all slip systems. Most crystal plasticity codes use empirical constitutive equations to describe these crystallographic shear rates. However, as crystal plasticity is build on dislocation motion and interaction, it is an obvious goal to introduce a constitutive model into such crystal plasticity FE codes which is based on dislocation densities as internal state variables. The dislocation model used in our approach is based on five main ingredients: 1) For every slip system mobile and immobile dislocations are distinguished. 2) The immobile dislocations are grouped into parallel and forest dislocations for each slip system. 3) A scaling relation between mobile and immobile dislocations is derived. 4) The Orowan equation is used as kinetic equation. 5) Rate equations for the immobile dislocation densities are formulated based on distinct dislocation processes, e.g. lock formation or annihilation by dislocation climb. Orientation gradients are implicitly described in terms of the dislocation density tensor. As a second set of constitutive models we introduce a physically based description of the mechanics of grain boundaries into the crystal plasticity FEM. While standard codes describe the grain boundaries as kinematical discontinuities (change of the orientation of the slip dyades between neighboring Gauss points) the new approach introduces a physically based model to map grain boundary mechanics in the FE model. Simulations will be shown for single as well as polycrystals and the results will be compared with experimental findings. Besides strain rate effects also the influence of temperature will be investigated.

8:45 AM EE4.2
Multiscale Study of FCC Bicrystals Deformation: Discrete Dislocation Dynamics and Continuum Gradient Crystal Plasticity. Firas Akasheh[1], Hussein Zbib[1] and Tetsyua Ohashi[2]; [1]Mechanical Engineering, Washington State University, Pullman, Washington; [2]Kitami Institute of Technology, Kitami, Japan.

The micromechanics of bicrystals deformation is of great interest for the current efforts to develop continuum crystal plasticity models that are more physics-based that are better capable of predicting the observed size dependant response of crystals on the micro scale. Furthermore, bicystals gain particular interest because they also serve as an idealized prototype model for the study of grain boundaries and their effect on the deformation of polycrystals. This work is an attempt along those efforts with particular focus on developing continuum models to describe the role of grain boundaries on mechanical response of polycrystals. Our approach is one of multiscale. On the micro scale discrete dislocation dynamics (DD) is used to simulate the physical behavior of dislocations as they interact with the bicrystal interface under the effect of the associated image forces. On the macroscale, a small strain crystal plasticity model, where dislocations are described as field densities, is used to simulate the same problem as that in DD. The evolution of dislocation densities, structure, as well as the mechanical response from both scales are compared. The parameters of the continuum model are fitted based on the results from DD, which is considered as the reference for comparison.

9:00 AM EE4.3
Discrete Dislocations Dynamics Investigation on Friction Damping under Cyclic Loading. Astrid Walcker[1], Daniel Weygand[1] and Oliver Kraft[1,2]; [1]Institut fuer Zuverlaessigkeit von Bauteilen und Systemen, Universitaet Karlsruhe (TH), Karlsruhe, Germany; [2]Institut fuer Materialforschung II, Forschungszentrum Karlsruhe, Karlsruhe, Germany.

The understanding of the small-scale mechanical response of metallic materials to ultra-high frequency cyclic loading conditions has been hardly studied in the past. For dislocations being the carriers of plastic deformation and, therefore, also of fatigue failure, the fundamental question concerns their behaviour under the influence of an oscillating stress. Beside its interesting fundamental aspects, this problem is also highly relevant for the reliability of thin metal films in MEMS or radio frequency communication devices. As the length scale of interest, i. e. a few hundred nanometers in film thickness, exceeds the computational realm of an atomistic simulation, this investigation is performed with a three-dimensional discrete dislocations dynamics (DDD) code, which has already been extensively tested and validated. A fcc crystal (Ni or Al) is subjected to an external stress oscillating harmonically with frequencies ranging from 1 MHz up to the GHz regime. The central quantity of interest is the frequency dependence of the dissipated mechanical work and its relationship with the materials properties (effective dislocation mass, shear modulus, damping coefficient) and the mobile dislocation length. The damping coefficient and the dislocation mass have been obtained from molecular dynamics simulations. In order to first clarify principal questions, a pinned single dislocation subjected to small stress amplitudes has been simulated. To verify the DDD simulations for ultra-high frequencies, an analytical model based on the equation of motion used by Granato and Luecke (1956) has been applied. The numerical results show a good agreement with the analytical solution. It turned out that for realistic damping values (of order 10$\hat{}$(-5) Pas at room temperature) and for the considered frequency range, the assumption of an overdamped regime is not justified and that the effective mass of the dislocation needs to be taken into account. Furthermore, a peak of the energy dissipation was found in the technically relevant GHz region. Based on these results, the present DDD simulations focus on the influence of the dislocation-dislocation interaction and of the distribution of loop lengths on the global dissipative response. As a transition between single and multi-dislocation configurations, different configurations with two dipolar dislocations are studied. For achieving a deeper understanding of cyclic deformation of thin metal films at ultra-high frequencies, configurations with randomly arranged dislocations are simulated.

9:15 AM EE4.4
Statistical Analysis of Dislocation Dynamics. Masato Hiratani and Vasily V. Bulatov; CMS/MSTD, Lawrence Livermore National Laboratory, Livermore, California.

Dislocation ensembles under various conditions are characterized by statistical analyses, and propagation of various physical information are examined. Raw data is obtained by using computational schemes of Langevin dislocation dynamics and deterministic dislocation dynamics. The strength of thermal agitations is determined to satisfy the equipartition law at any time and length scale of interest under relaxation. In creep simulations of dislocation percolation in irradiated copper, the correlation of dislocation kinetic energy is found to be rapidly decaying over time and space, and strongly temperature dependent. As temperature decreases, the energy correlation is elongated, eventually exceeds the length scale of some microstructures (e.g. average local defect spacing), and results in dislocation evolution completely different from that of overdumped system. In constant strain rate simulations of nickel and molybdenum, our fractal analysis indicates that the correlation of stress fluctuations is slowly decaying (power law) at low rate regimes. Correspondingly, dislocation-dislocation interactive forces are observed to be dominant at the low rate regimes while the role of external forces becomes larger at high rate regimes. Based on given analyses, some attempt to build a further coarse-grained continuum model will be also presented. This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

9:30 AM EE4.5
Competing Length Scales in Metallic Multilayer Thin Films. Peter M. Anderson, Dept of Materials Science and Engineeering, Ohio State University, Columbus, Ohio.

The extraordinary strength of nanostructured materials is attributed to the confinement of slip to small volumes. For metallic multilayer thin films, the small volume corresponds to individual layers. In this regime, dislocation-based theories predict plastic strength to scale approximately as 1/layer thickness for single pile-up and 1/(layer thickness)$\hat{}$0.5 for multiple-dislocation pile-ups. However, below a critical layer thickness, slip can not be confined to individual layer thickness, so that the small volume is controlled by a new length scale. Candidates for this new length scale are the critical layer thickness and a dislocation source length. In principle, both of these length scales are controlled by interfacial properties that dictate barrier strengths to dislocation transmission as well as critical conditions for loop nucleation. A cellular automaton dislocation model is employed to study the effect of layer thickness, barrier strength, and interfacial source length on the plastic strength of multilayer thin films. The model results are compared to experimental data to provide insight on the competition between these length scales in specific multilayer thin films systems.

9:45 AM EE4.6
Dislocation Core Properties of Ni-Cu Nanolaminates: An Ab Initio-Based Study. Wei Xiao[1], Nicholas Kioussis[1], Gang Lu[1] and Nasr Ghoniem[2]; [1]Physics, California State University Northridge, Northridge, California; [2]Mechanical and Aerospace Engineering, University of California Los Angeles, Los Angeles, California.

Metallic multilayered structures have received increasingly interest in the past few years because of their unusual and interesting mechanical properties and high strength-to-weight ratio. The mechanical properties of an interface are determined, in large part, by the nature of the chemical bonding at the interface, which may be significantly different from that within either of the materials meeting at the interface. The resistance of interfaces to dislocation transmission is a fundamental quantity that often serves to control strength in plastically deforming multiphase materials. We have generalized an mutliscale approach based on semidiscrete variational generalized Peierls-Nabarro (SVGPN) model to study the dislocation core properties of Ni-Cu nanolaminates. The generalized stacking fault energy surfaces (GSFES) for the pure Cu, Ni, and the (001) Ni-Cu interface have been calculated from ab initio calculations. Various dislocation properties, such as the core width, energy, the Peierls stress, the dissociation behavior are investigated and compared to those of the pure Cu and Ni hosts. Supported bu US Air Force grant 0205GDD417

10:30 AM *EE4.7
Robust Quantum-Based Interatomic Potentials for Multiscale Modeling in Transition Metals. John A. Moriarty, Lawrence Livermore National Laboratory, Livermore, California.

First-principles generalized pseudopotential theory (GPT) provides a fundamental basis for transferable multi-ion interatomic potentials in transition metals and alloys within density-functional quantum mechanics. In central bcc transition metals, where multi-ion angular forces are important to structural properties, simplified model GPT or MGPT potentials have been developed based on canonical d bands to allow analytic forms and large-scale atomistic simulations. Robust, advanced-generation MGPT potentials have now been obtained for Ta and Mo and successfully applied to a wide range of structural, thermodynamic, defect and mechanical properties at both ambient and extreme conditions, including multiphase equation of state, melting and rapid resolidification, thermoelasticity and detailed atomistic simulations of point defects, dislocations and grain boundaries needed for the multiscale modeling of plasticity and strength. Recent algorithm improvements have allowed more general matrix representations beyond canonical bands for increased accuracy and extension to f-electron actinide metals, as well as a factor of six increase in computational speed. Further developments in progress include temperature-dependent potentials, the treatment of correlated electrons beyond density functional theory, and the retention of higher multi-ion interactions. This work was performed under the auspices of the U.S. Dept. of Energy by the University of California Lawrence Livermore National Lab. under contract No. W-7405-E

11:00 AM EE4.8
Nanoscale Twinning and Martensitic Transformation in Shock-Deformed BCC Metals. Luke L. Hsiung, Chemistry and Materials Science, Lawrence Livermore National Laboratory, Livermore, California.

Shock-induced twinning and martensitic transformation in BCC-based metals and alloys (Ta, Ta-W, and U6Nb) have been observed and studied using transmission electron microscopy (TEM). The length-scale of domain thickness for both twin lamella and martensite phase is found to be smaller than 100 nm. While deformation twinning of {112}<111>-type is found to occur in Ta when shock-deformed at 15 GPa, martensitic transformation is found to occur when shock-deformed at 45 GPa. Similar phenomena of nano-scale twinning and martensitic transformation are also found within U6Nb shock-deformed at 30 GPa. Since both deformation twinning and martensitic transformation occurred along the {211}b planes associated with high resolved shear stresses, it is suggested

that both can be regarded as alternative paths for shear transformations occurred in shock-deformed BCC metals. Dynamic dislocation mechanisms and critical stresses for the nucleation of shock-induced twinning and martensitic transformation are proposed and discussed. This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

11:15 AM EE4.9
First-Principles Calculations of Mechanical Properties of Aluminum Oxycarbide Al2OC. Rong Yu[1], Xiao Feng Zhang[1], Rowland M. Cannon[1], Lutgard C. De Jonghe[1,2] and Robert O. Ritchie[1,2]; [1]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California; [2]Department of Materials Science and Engineering, University of California, Berkeley, Berkeley, California.

Al2OC-based intergranular layers will form in SiC polycrystals when processed with Al, B, and C additives (ABC?SiC). Various mechanical tests on hot presses ABC-SiC implied a profound influence of the interface layers on mechanical performance at ambient and elevated temperatures. However, because of the 1 nm thickness of the Al2OC intergranular layers, experimental determination of their mechanical properties is difficult. In this study, the mechanical properties of Al2OC were computed from first-principles and compared with those of 2H-SiC. The crystal structure of Al2OC is based on the hexagonal wurtzite structure. An ordered structure model was adopted. The calculations were performed using local density functional theory. Structural optimization and mechanical properties were calculated. The bulk modulus, Young's modulus and theoretical strength in [001] direction of Al2OC and of 2H-SiC were calculated. The theoretical strength of Al2OC was found to be about one half of that of SiC. This may provide an explanation for the improved toughness of the ABC-SiC samples, as a consequence of fracture propagating along the weaker Al2OC grain boundary films.

11:30 AM EE4.10
Electronic Theory for Embrittlement of Grain Boundaries in Ni3Al. Dipanjan Sen[1], Wolfgang Windl[1], Gerd Duscher[2,3] and Matthew Chisholm[3]; [1]Dept. of Materials Science and Engineering, The Ohio State University, Columbus, Ohio; [2]Dept. of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina; [3]Condensed Matter Science Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Catastrophic brittle fracture of crystalline materials is among the best documented but least understood fundamental phenomena in materials science. Modern computational methods such as density-functional ab-initio calculations are in principle capable to study the effect of segregants on bonding and electronic structure and give answers to these questions. However, the results depend strongly on the detailed structure of the grain boundary, and knowledge of the exact structure is a necessity for sensible results. In this study, we use a combination of aberration-corrected atomic resolution Z-contrast imaging, electron and energy-loss spectroscopy as well as atomistic modeling based on the embedded-atom method (EAM) and density-functional theory (DFT) to investigate, at the atomic scale, the geometric and electronic structure of metal grain boundaries with and without segregants. A feature common to the majority of brittle fractures is the segregation of impurity elements to the grain boundaries of the material. Losch first proposed the idea that impurity-induced changes to the electronic structure could be responsible for the macroscopic loss of ductility in metals. The numerous electronic structure calculations that followed this seminal work have resulted in several proposed mechanisms of embrittlement. However, we find that these theories cannot satisfactorily explain the situation for our system under investigation, B and H segregated to Ni3Al grain boundaries. In the theory we propose, the bonding at the grain boundaries is a function of localized electron depletion or accumulation and can be evaluated by examining the deviation of the electron density at the boundary from the (optimum) bulk electron density in comparison to stress/strain studies using a combination of EAM and DFT. The EAM simulations allow us to study large simulation cells with and without finite temperature, where we can keep the grain boundaries far apart from each other. We then use DFT to zoom in on the bonding at grain boundaries with and without segregants and to calculate electron-density difference plots and Bader-type charge maps.

11:45 AM EE4.11
Multiscale Characterization of Deformation Mechanisms in the Weld Joint of a Ni-Based Superalloy. Oleg M. Barabash, Joe A. Horton, Suresh S. Babu, John M. Vitek, Stan A. David, Gene E. Ice and Rozaliya I. Barabash; Metals and Ceramics Div., Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Multiscale plastic deformation in the heat affected zone (HAZ) of a Ni-based single crystal superalloy has been characterized using white microbeam synchrotron diffraction measurements together with OIM imaging, electron and optical microscopy. Characteristic length scales on the macro, meso and nano scale are determined. Dissolution of the γ' - phase particles during heating and secondary precipitation of γ' during cooling is found, as well as formation and multiplication of dislocations. This process is more intense as one approaches the fusion line (FL). In the regions immediately neighboring the FL, γ' - phase particles dissolve completely and re-precipitate from the solid solution in the form of very small (10-20nm) particles. In the immediate vicinity of the FL, the temperature gradient and the rate of it's change reaches maximal values and causes the formation of large amounts of dislocations. Dislocations are concentrated in the γ matrix of the single crystal superalloy. X-ray Laue diffraction (both conventional and microbeam) and electron microscopy show that alternating dislocations slip systems dominate in the HAZ with Burgers vector b=[110] and dislocation lines [1-12] and [1-1-2]; or b=[-110] , dislocation lines [112] and [11-2] . Each of these two dislocation groups forms Z-shaped dislocation lines fluctuating around two cubic directions [100] and [010]. Local lattice rotations in different zones of the weld joint are linking with the microslip events in different zones of the weld.

SESSION EE5: Time and Length Scales for Microstructural Heterogeneity and Radiation Damage
Chairs: Wolfgang Windl and Dieter Wolf
Wednesday Afternoon, March 30, 2005
Room 2018 (Moscone West)

1:30 PM *EE5.1
Microstructurally Informed Elasticity, Plasticity and Failure. Elizabeth A. Holm, Corbett C. Battaile, Thomas E. Buchheit, Michael K. Neilsen, Gerald W. Wellman and Kristopher Healey; Materials and Process Modeling, Sandia National Laboratory, Albuquerque, New Mexico.

The fundamental premise of materials science is that composition isn't everything. From its earliest days, materials science has been concerned with how fine-scale structures alter the properties of materials. This is the guiding principle behind the study of microstructure, including dislocations, grains, phases, defects, flaws, and precipitates. In this talk, we will discuss computational approaches to incorporating microstructure into property predictions. In some cases, it is sufficient to include a microstructural parameter in the constitutive relations for material behavior, as in a continuum plasticity model. In others, the microstructure must be included explicitly, for example, when predicting elastic failure nucleation or the morphology of a brittle fracture surface. Finally, during material processing, microstructural evolution may depend on material properties, and vice versa. For processes such as plastic forming or recrystallization, coupled microstructural and micromechanical models can provide new insight. Using approaches such as these, computational materials science follows the scientific tenet of materials science: to understand the interdependence of composition, structure, processing, and performance. This work was performed in part at Sandia National Laboratories, a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

2:00 PM EE5.2
Characterization of the Microstructure and Strengthening Mechanisms in a Cryomilled Al 5083 Alloy. Gene Lucadamo[1], Nancy Y. C. Yang[1], Chris W. San Marchi[1] and Enrique J. Lavernia[2]; [1]Sandia National Laboratories, Livermore, California; [2]University of California, Davis, Davis, California.

Cryomilling generates nanostructured powders from a range of starting metals and alloys. In this work, we investigate the microstructure and mechanical properties of an Al 5083 alloy (4 wt.% Mg, 0.5 wt.% Mn, 0.07 wt.% Cr) following cryomilling, hot isostatic pressing (HIP), and extrusion. This process can yield alloys with high strength and low weight. The vickers hardness of the material formed using the cryomilled 5083 Al powder is three times that of wrought 5083 Al($\leq$60VHN). Our initial studies identify several sources of strengthening. These include: sub-micron grain sizes in the as-extruded material, $MnAl_6$ dispersoids, fine precipitates, and incorporated metal-oxide phases resulting from the milling process. Also, the Mg in the alloy is expected to produce some solid solution strengthening. Using complementary transmission electron microscopy (TEM) techniques such as energy filtered (EFTEM) and weak beam imaging, we characterize the microstructure to understand the mechanisms responsible for the increased hardness. Diffraction contrast TEM images indicate strong interactions between lattice dislocations and the second phases. Our current efforts involve quantifying the relative contributions of these mechanisms to the

measured mechanical response. In addition to the study of the as-processed material, preliminary results from heat treated specimens indicate that the room temperature microhardness essentially is unchanged following annealing at temperatures that approach 0.8 Tm. Continued precipitation and grain boundary pinning by oxide particles and nitrides at elevated temperatures may account for the persistence of strength. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

2:15 PM EE5.3
Dislocation-Induced Crossover Scaling During Spinodal Decomposition. Mikko P. Haataja[1], Jennifer Mahon[2], Nikolas Provatas[2] and Francois Leonard[3]; [1]Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey; [2]Materials Science and Engineering, McMaster University, Hamilton, Ontario, Canada; [3]Sandia National Laboratories, Livermore, California.

Spinodal decomposition is a technologically important solid-solid phase transformation which is often employed to strengthen alloys. A particularly interesting aspect of this process is the interaction between dislocations and evolving microstructure in lattice mismatched alloys, where the development of microstructure is accompanied by a build-up of elastic coherency strains. At late times, thermodynamic considerations imply that misfit dislocations will migrate to the compositional domain walls and relax the coherency strains. Such considerations alone, however, are insufficient to describe the strongly coupled evolution of the compositional domains and dislocations. Here we examine the effects of mobile dislocations on spinodal decomposition kinetics and subsequent coarsening in lattice mismatched binary alloys. By employing a novel continuum model, which incorporates dislocation discreteness effects, we demonstrate that the effects of dislocation mobility on domain coarsening kinetics can be expressed in a unified manner through a scaling function. Our prediction is amenable to direct experimental verification.

EE5.4
Abstract Withdrawn

2:30 PM EE5.5
Modeling the Influence of Microscale Heterogeneity on the Macroscale Failure of Multiphase Materials. Jeremy Leggoe, Chemical Engineering, Texas Tech University, Lubbock, Texas.

Spatial heterogeneity in the distribution of secondary phases can exert a profound influence on the macroscopic properties of multiphase materials. Spatial heterogeneity is typically induced during material synthesis, with interdendritic segregation of the introduced phase being a particular problem for melt cast composites. Local matrix variations, combined with the prevalence of failure nucleation sites and the complex stress states arising within particle clusters, can adversely influence the fracture properties of polymer and metal matrix composites. A Cellular Automata (CA) approach has been adapted to provide a multi-scale approach to investigating the effect of spatial heterogeneity on failure in ductile alloys and particulate reinforced metal matrix composite materials. As the spatial distribution of the initial porosity deviates from the homogeneous ideal, the strain field developing within the models becomes increasingly heterogeneous, the effect being most pronounced at high strains. The variability of the macroscale response similarly increased as the initial porosity distribution deviated from homogeneity, with variation being most evident as the models approach failure. The stress supported declined significantly as the initial porosity distribution became increasingly heterogeneous, indicating that the severity of local property disparities plays an important role in the process of strain localization and final failure. Advances in the development of multiscale failure models are dependent on the development of techniques for accurately characterizing the nature of spatial heterogeneity, so that it may be realistically recreated in computational simulations. A variety of measures of disorder or heterogeneity have been developed that compare the short-range characteristics of particle distributions with those of random particle dispersions, such as nearest neighbor statistics or Pair-Distribution functions. Care must be taken, however, that such measures are based on comparisons with appropriate dispersions; particle dispersions are not Poisson point processes, and polydispersity can substantially influence nearest neighbor statistics. This investigation is developing Nth nearest neighbor statistics as a tool for characterizing the extent and length scale of clustering in materials containing dispersed secondary phase particles. Consideration is given to the influence of the form in which the particle distribution is characterized on the data collected; 2D microstructure representations can yield statistics varying significantly from those of the actual three dimensional structure. The development of physically based forms of heterogeneous spatial distribution recreation, such as the placement of repulsive nodes to generate three dimensional necklaced particle structures representative of interdendritic segregation, will also be discussed in this presentation.

3:30 PM *EE5.6
Linking Time and Length Scales in the Modeling of Radiation Damage in Model Ceramics. Blas Pedro Uberuaga, Los Alamos National Laboratory, Los Alamos, New Mexico.

Studying the effect of radiation damage in ceramic materials is of interest for understanding and improving their potential uses in irradiated environments, such as in nuclear reactor walls and windows, nuclear fuel encapsulation, and nuclear waste disposal. Molecular dynamics (MD) is ideally suited for simulating a primary knock-on event, which generates a cascade region in a few ps. However, the ultimate microstructural response of the material (e.g., amorphization, void growth, dislocation formation, etc.) typically depends in a critical way on diffusive processes taking place on a much longer time scale, inaccessible to direct MD. The recently developed temperature accelerated dynamics (TAD) method offers a way to simulate the diffusive behavior of the complex defects accurately on these longer time scales (e.g., ms, s), without making prior assumptions about the diffusion mechanisms or the way the defects might combine and evolve. We present results on low-energy cascades (e.g., 0.4 to 5 keV) in MgO and MgAl2O4 spinel, using MD to simulate the cascade dynamics for a few ps. We then use TAD to study the diffusion and evolution of the defects formed in the cascades on much longer times scales, and molecular statics to probe the stability of various defects (e.g., interstitial clusters, vacancy clusters) that may dominate at long times. An interesting picture emerges for MgO, with large (containing 6 atoms) interstitial clusters being surprisingly mobile. Using these atomic scale results as a basis, we have developed an initial kinetic rate theory model to describe the formation of dislocation loops in MgO, where we see an impact of the mobile interstitial clusters on predicted loop size. Preliminary results on Al-doped MgO and spinel will also be presented.

4:00 PM EE5.7
Multiscale Modeling of Radiation Damage in Neutron Irradiated SiC. Behrooz Khorsandi[1], Thomas E. Blue[1] and Wolfgang Windl[2]; [1]Nuclear Engineering, The Ohio State Univeristy, Columbus, Ohio; [2]Materials Science & Engineering, The Ohio State University, Columbus, Ohio.

Silicon carbide is a highly suitable semiconductor material for applications in environments with extreme temperature and irradiation due to its wide band gap and radiation hardness. These properties make SiC a potential candidate for semiconductor-based neutron flux monitors in nuclear reactors. Despite its radiation hardness, the properties of SiC will be affected by energetic neutron irradiation at sufficient energy and dose, resulting in vacancies, interstitials, antisites and their complexes. This damage in turn can deteriorate the electrical properties and may eventually lead to failure of the device. In this paper, we will examine radiation damage in 4H-SiC due to neutron irradiation and try to predict the deterioration of its properties and ultimately the theoretical lifetime of the device in a reactor environment. To the best of our knowledge, there is no single program that can model the impact of neutron irradiation on displacement damage of SiC. However, programs exist to model the conditional probability for a neutron to interact with a Si or C atom (e.g., MCNP5 [MCNP: A General Monte Carlo N-Particle Transport Code, Version 5, Los Alamos National Laboratory, Los Alamos, NM (2003)]) and to model the damage evolution, once the energy and direction of a SiC atom accelerated by a neutron (a so-called primary knock-on atom (PKA)) is known (e.g., TRIM [http://www.srim.org]). Thus, we have developed a MATLAB program to determine the PKA specifications (type, energy, position and direction) from the MCNP5 output and used it as an input for TRIM to predict the number of displacements. With our methodology, we can currently predict the instantaneous damage in neutron-irradiated SiC detectors with typical dimensions (several hundred um lateral dimensions and 10 um thickness). Our current work is to develop a continuum model of the damage evolution between neutron impacts based on ab-initio parameters, enabling us to model the effect of irradiation from short times to continuous exposure upon integration of the different programs into a common platform. For this, we combine classical molecular dynamics simulations based on a Tersoff potential with ab-initio calculations of diffusion and reaction barriers, which serve as input to a partial-differential equation system for the concentrations of the defects and defect clusters, similar to previous work on damage evolution in ion-implanted Si [X. Y. Liu, W. Windl, and M. P. Masquelier, Appl. Phys. Lett. 77, 2018 (2000)]. This material is based upon work supported by the US Department of Energy under the NERI program Award No. DE-FG-07-02SF22620 and NERI Project Number 02-207. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the Department of Energy.

4:15 PM EE5.8
Simulations of the Effects Helium and Hydrogen in Iron Subjected to Irradiation Damage. Maria A. Okuniewski[1], Chaitanya S. Deo[2], Srinivasan G. Srivilliputhur[2], Mike I. Baskes[2], Stuart A. Maloy[2], Michael R. James[2] and James F. Stubbins[1]; [1]Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois; [2]Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, New Mexico.

High-energy neutrons produce displacement damage as well as introduce gaseous transmutation products (helium and hydrogen) in nuclear reactor structural materials. The displacement damage as well as the introduction of helium and hydrogen can interact dynamically, leading to altered mechanical behavior. Modeling can help to understand this change in behavior and to evaluate new potential nuclear reactor materials. A multi-scale modeling effort employing molecular dynamics (MD) and kinetic Monte Carlo (kMC) simulations is underway to study these effects of helium and hydrogen in irradiated body-centered cubic (bcc) iron. The results obtained from the MD work will be utilized to parameterize the input for the kMC simulations. The kMC results will provide defect evolution on much larger length and time scales than the MD results. This paper will focus on the MD work conducted. A systematic study of irradiation processes in pure bcc iron, iron-helium, and iron-hydrogen will be carried out to examine the atomistics and characterize the defect evolution. The effects of incident ion energies, helium and hydrogen concentrations, and temperatures on the evolution of defects, including helium and hydrogen interstitials, clusters, and bubbles are investigated. The modified embedded atom method potential, which is based on the density functional theory and explicitly incorporates angular forces that are essential to model the iron-helium and iron-hydrogen systems, is used.

4:30 PM EE5.9
Kinetic Monte Carlo Simulations of Helium and Hydrogen Clustering in Radiation Damaged Iron. Chaitanya Suresh Deo[1], Srinivasan Srivilliputhur[1], Michael Baskes[1], Stuart Maloy[1], Michael James[3], Maria Okuniewski[2] and James Stubbins[2]; [1]MST-8, Los Alamos National Laboratory, Los Alamos, New Mexico; [2]Dept. of Nuclear Engineering, University of Illilois, Urbana Champaign, Illinois; [3]D-5, Los Alamos National Laboratory, Los Alamos, New Mexico.

Micro-structural defects are introduced in materials upon irradiation with energetic particles. These defects can cause degradation of mechanical properties and contribute to material failure. Transmutation products such as hydrogen and helium in irradiated stainless steels exert deleterious effects on material properties. A description of the atomic mechanisms governing the process and their correlation to material properties will result in better understanding of the mechanisms by which iron and iron-based alloys respond to helium and hydrogen implantation by radiation and will suggest methods of alloy improvement to withstand irradiation damage. We have performed kinetic Monte Carlo (KMC) simulations of point defect diffusion and clustering in bcc alpha iron. The model consists of the following entities in bcc iron: interstitial and substitutional helium and hydrogen atoms, interstitial iron atoms, vacancies, vacancy-clusters, and sinks for the trapping of point defects (dislocations and grain boundaries). Input to the simulations includes the migration energies of the point defects (interstitial iron, vacancy, interstitial and substitutional helium and hydrogen), formation energies of the HenVm clusters, dissociation energies of the point defects from the HenVm clusters and initial concentrations and configurations of point defects and defect ratios. These quantities are obtained from experimental data, molecular dynamics (MD) simulations using embedded atom and modified embedded atom potentials. The defect ratios and configurations can obtained from the post-cascade data of large MD runs. We employ the KMC simulations to investigate the time evolution of the point defect configuration leading to defect clustering and bubble formation. The composition of embryonic defect clusters as a function of time and operating temperatures is determined. It is found that almost all the transmuted helium and hydrogen is trapped in sink configurations (clusters, dislocations or grain boundaries) within a fraction of a microsecond.

4:45 PM EE5.10
Atomic-scale Contribution to Understanding Mechanical Properties of Irradiated Metals. Yury Osetskiy[1], Roger E. Stoller[2] and David J. Bacon[3]; [1]Computer Sciences and Math, ORNL, Oak Ridge, Tennessee; [2]Metals and Ceramics, ORNL, Oak Ridge, Tennessee; [3]Engineering, The University of Liverpool, Liverpool, United Kingdom.

The present paper reports recent progress in atomic-level dislocation dynamics achieved by exploring large-scale simulation of realistic dislocation and radiation induced defects (voids, precipitates and stacking fault tetrahedra (SFTs)) densities. We have considered gliding edge and screw dislocations interacting with obstacles of size of up to 12nm over the temperature range from 0 to 600K. A variety of different reactions have been observed, such as dislocation climb, cross-slip and formation of superjogs at the dislocation line and obstacle modification. These cannot be rationalized without taking into account specific atomic-scale structure of dislocations and SFTs. The atomic-scale mechanisms observed are discussed and tentative interpretation of some experimental results is given.

SESSION EE6/BB6: Joint Session: Linking Length Scales in the Mechanical Behavior of Materials
Chairs: John Balk and Daniel Weygand
Thursday Morning, March 31, 2005
Room 2016 (Moscone West)

8:30 AM *EE6.1/BB6.1
Interplay between High-temperature Deformation and Grain Growth in Nanocrystalline Materials by Hierarchical Multiscale Simulation. Dieter Wolf[1], Andrew Haslam[2], Vesselin Yamakov[3], Dorel Moldovan[4], Rong Ding[1] and Simon Phillpot[5]; [1]Materials Science Div., Argonne Natl Lab, Argonne, Illinois; [2]Dept. of Chem. Engrg., Imperial College, London, United Kingdom; [3]National Institute of Aerospace, Hampton, Virginia; [4]Dept. of Mechanical Engrg., Louisiana State University, Baton Rouge, Louisiana; [5]Dept. of Materials Science and Engrg., University of Florida, Gainesville, Florida.

Molecular-dynamics simulations have been used to elucidate the intricate, highly non-linear coupling between grain-boundary diffusion creep and grain growth in nanocrystalline metals. We demonstrate how the materials-physics based insights into the underlying deformation and grain-growth growth mechanisms extracted from these simulations can be rigorously incorporated into a mesoscopic simulation model, thus overcoming the length and time-scale limitations inherent to the MD approach. The objects evolving in space and time in the mesoscale simulations are the discretized grain boundaries and grain junctions rather than the atoms themselves, involving characteristic length and time scales governed by grain-boundary processes and parameters rather than atom vibrations. This then enables analysis of the intricate interplay between grain growth and grain-boundary diffusion creep for a system containing a large number of grains with arbitrary sizes.
Work supported by the U.S. Department of Energy, Basic Energy Sciences-Materials Sciences, under Contract W-31-109-Eng-38.

9:00 AM EE6.2/BB6.2
Atomistic Modelling of Interactions between Lattice Dislocations and Grain Boundaries in Body-centered Cubic Transition Metals. Matous Mrovec[1], Christian Elsaesser[1] and Gumbsch Peter[1,2]; [1]Fraunhofer-Institut fuer Werkstoffmechanik, Freiburg, Germany; [2]Institut fuer Zuverlaessigkeit von Bauteilen und Systemen, Universitaet Karlsruhe, Karlsruhe, Germany.

With grain sizes decreasing towards the nanometer scale, the plastic deformability of polycrystalline metals is increasingly controlled by interactions between lattice dislocations and grain boundaries. In order to elucidate atomic-level mechanisms and processes of such interactions, computer simulations were carried out for atomistic models of dislocations interacting with boundaries in body-centered cubic (bcc) transition metals. The interatomic interactions were described by real-space bond-order potentials (BOP) derived from tight-binding electronic-structure theory [1]. These recently developed BOP have been applied already with success to simulate atomistic core structures of individual screw dislocations [2] and twin boundaries [3] in molybdenum, tungsten and other bcc metals. In this contribution, BOP simulation results will be presented for atomistic structures and mechanical responses of tungsten bicrystal models containing a twin boundary and a screw dislocation. [1] M. Mrovec, PhD Thesis, University of Pennsylvania, Philadelphia (2002). [2] M. Mrovec, D. Nguyen-Manh, V. Vitek, D. G. Pettifor, Phys. Rev. B 69, 095115 (2004). [3] T. Ochs, C. Elsaesser, M. Mrovec, V. Vitek, J. Belak, J. A. Moriarty, Phil. Mag. A 80, 2405 (2000).

9:15 AM EE6.3/BB6.3
The Nature of Slip in Deformation Simulations of Metallic Nanocrystalline Materials. Helena Van Swygenhoven, Anders Froseth and Peter M. Derlet; ASQ/NUM, Paul Scherrer Institution, Villigen PSI, Switzerland.

Slip in molecular dynamics simulations of fcc nanocrystalline materials is mediated by partial dislocations nucleated and absorbed at grain boundary regions. The ultimate nature of this slip, whether it be extended partials, full dislocations or twin faulting has recently be

shown to depend on the general planar fault energy curves of the corresponding metal. In order to fully understand the detailed process of full dislocation activity as observed in MD simulations of nc-metals a more elaborate theory based on the dislocation nucleation process, the curved character of the dislocation, the GB structure of the nucleation site and the interactions of the dislocations with the GB has to be developed. In the present work we show that the splitting distance of the dissociated full dislocation cannot account for the correct nucleation physics of the leading and trailing partial dislocations. Even once both partial dislocations are nucleated, the local stress distribution plays an important role in the separation of the partials. Furthermore, by means of a detailed temporal output of energy, crystallinity and local averaged stress, we present a detailed analysis of the stress distribution and evolution in the GBs during emission of the dislocations allowing to pin down the important parameters of the nucleation and absorption processes of dislocations from GBs. We request that this submission be considered in the joint session between BB and EE

9:30 AM EE6.4/BB6.4

Developing Experimentally-Tuned Grain Boundary Networks for use in Molecular Dynamics Simulations. Anders Froseth, Peter M. Derlet and Helena Van Swygenhoven; ASQ/NUM, Paul Scherrer Institution, Villigen PSI, Switzerland.

It is well known from experimental observations that not only the grain size but also the type of grain boundary (GB) network greatly influences the mechanical response of nanocrystalline (nc) metals. Detailed information on an optimal GB network is however lacking. Until now, Molecular Dynamics (MD) deformation simulations of 3D-nanocrystalline metals have mainly been performed for a relatively small number of grains using the Voronoi construction and random grain orientations. We have developed a method using a combined Voronoi/Delaunay technique to geometrically construct samples with a pre-selected number of special GBs. Motivated by TEM observations of nc materials we employ this method to fine-tune simulated GB networks to more realistically represent known experimental structures. We present results for a series of nc-Ni samples containing 200 grains with a pre-selected number of either special symmetric low angle boundaries, or carefully selected Coincidence Site Lattice (CSL) boundaries. We demonstrate how special GB networks respond differently to plastic deformation compared to GB networks containing random grain orientations, give details on the activated deformation mechanism and draw conclusions concerning experimental observations. We request that this submission be considered for the joint session between EE and BB

9:45 AM EE6.5/BB6.5

The Impact of Length and Time Scale Limitations on Solute Drag Theory During Experiment and Modelling of Recrystallization in Aluminum Alloys. Mitra L. Taheri[1], Eric Stach[2], Velimir Radmilovic[3], Hasso Weiland[4] and Anthony D. Rollett[1]; [1]Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania; [2]Materials Science and Engineering, Purdue University, West Lafayette, Indiana; [3]National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, California; [4]Alcoa Technical Center, Alcoa Center, Pennsylvania.

The effect of solutes on the migration of boundaries has long been a topic of investigation due to its tremendous impact on its applications in materials science, both industrial and academic. The lack of measurement of the solute drag effect can be attributed in part to the limitations of current imaging capabilities of electron microscopes. Thus, there exists a limited amount of experimental investigation with respect to solute drag, all of which has been performed using scanning and transmission electron microscopy, regardless of their respective inadequacies. Evidence of both solute drag as well as differences in growth mechanisms of certain boundary types has been noted in both current literature and the results presented herein for an Aluminum-Zirconium alloy system. Recently, there have been indications of the limitations of scanning electron microscopy on the length and time scale of these experiments. New theoretical developments suggest that boundary motion should be jerky. This suggestion emerged from extensive computer simulation, together with new theory, and is supported by results from in-situ annealing experiments within a scanning electron microscope. In response to these findings, in-situ annealing experiments within a transmission electron microscope have shown a stark contrast between solute segregation at small scales and large scales; these experiments were coupled with Z contrast imaging and energy dispersive spectroscopy to locate solute segregation. Specifically, Zr was found to segregate to Al boundaries at grain sizes of approximately 2 microns and not at boundaries for grains of diameters of 20 microns or larger, suggesting a boundary breakaway phenomenon directly related to length and time scales during annealing. In addition, Zr was found to inhibit specific boundary types, promoting mobile 111 tilt boundaries due to strong segregation to twist boundaries. This as well as segregation with respect to boundary morphology and character during recrystallization are presented in this paper.

10:30 AM *EE6.6/BB6.6

Modelling Hardening Behaviour and Dislocation Grain Boundary Interaction in Thin Films. Peter Gumbsch[1,2], Daniel Weygand[1,2] and Zhaohui Jin[1]; [1]University of Karlsruhe, Karlsruhe, Germany; [2]Fraunhofer IWM, Freiburg, Germany.

The plastic deformation of polycrystalline fcc metal thin films is investigated by simulating the dynamics of discrete dislocations in a representative columnar grain. The simulations are based on the assumption that dislocation sources or multiplication sites are rare and that sources have to operate several times to generate appreciable plastic deformation. The work hardening of such thin films, the influence of boundary conditions and the evolution of dislocation densities are studied. In particular, the interaction of a dislocation with forest dislocations leads to different types of sessile or glissile lock. While the former have already attracted much attention, the behavior of the glissile lock, which can change the character of a dislocation in its glide plane, has not yet been investigated in detail by simulation. The discrete dislocation dynamics simulations results show, that the glissile lock is an effective dislocation source, which allows populating a new slip system that has not been activated before. As this multiplication mechanism is completely athermal, it is a possible stress relaxation mechanism for thin films at low temperatures where thermally activated cross-slip is becoming unlikely. Another important stress relaxation mechanism in thin films and nanostructured materials is dislocation passage through grain boundaries or (re)nucleation of dislocations from grain boundaries. Atomistic simulations are applied to study these processes. In particular, the strength of heavily twinned materials is analyzed in terms of dislocation-twin boundary interaction.

11:00 AM *EE6.7/BB6.7

Quantitative Modeling at the Nanoscale. Lyle Levine, F. Tavazza, L. Ma, R. Wagner and A. M. Chaka; NIST, Gaithersburg, Maryland.

Device design at the nanoscale is inherently multiscale and is further complicated by a lack of modeling tools with quantifiable uncertainties. For example, in determining the operational elastic limits of a proposed nanoscale device, the macroscopic stresses on the device must be propagated down to the individual atoms where the first dislocation or crack initiates. Making such simulations quantitative is extremely challenging by itself, but setting up methodologies that can be used routinely by device designers adds even more constraints. To bridge the relevant length scales, we are using finite element modeling (FEM) to model the macroscopic geometry of nanomechanics experiments, with an initial emphasis on nanoindentation. The FEM mesh refines down to individual atom positions, allowing elastic displacements to be directly propagated to localized atomistic simulations that use classical potentials. In the vicinity of the first inelastic event, bond distortions become large and classical potentials cannot be used for quantitative predictions. For these atoms, we have developed a hybrid quantum-classical algorithm for embedding a quantitative, all-electron, quantum mechanics-based simulation within the larger classical potential region. Validation testing requires quantitative topographic measurements of the indenter tip and the sample surface before contact and quantitative measurements of sub-nanoNewton forces. Specific validated simulations will be developed as Standard Reference Simulations that device designers can use to calibrate their own modeling predictions.

11:30 AM EE6.8/BB6.8

Direct Calculation of Stiffness and Mobility of Flat Grain Boundaries - Atomistic Simulations. Moneesh Upmanyu[1] and Zachary T. Trautt[2]; [1]Engineering Division, Materials Science Program, Colorado School of Mines, Golden, Colorado; [2]Engineering Division, Colorado School of Mines, Golden, Colorado.

Dislocation-grain boundary interactions play an important role in recrystallization and deformation of polycrystalline materials. In most multi-scale approaches, the induced motion of grain boundaries is assumed to be proportional to the dislocation density gradients, and the grain boundary stiffness is approximated to be equal to the grain boundary free energy. Here, we present molecular dynamics simulations at extracting grain boundary stiffness during motion induced explicity by dislocation density gradients. The capillarity forces acting on grain boundaries depend on their stiffness. In this study, we perform molecular dynamics (MD) simulations of capillarity induced fluctuations in grain boundaries with inclination dependent grain boundary energies aimed at extracting their stiffness. The simulations are performed in triangular lattice Lennard-Jones model system at T=0.3T_m, for two symmetric tilt grain boundaries with

identical inclinations and misorientations. Both boundaries exhibit a well-defined fluctuation spectrum. Analysis of the fluctuation spectrum of the high symmetry boundary reveals that its spectral content is consistent with capillarity wave theory, and the calculated grain boundary stiffness is significantly higher that the free energy of a corresponding asymmetric tilt grain boundary. On the other hand, the fluctuation spectrum of a low symmetry boundary exhibits peaks at certain modes, and the boundary is not rough. Plot of the equilibrium grain boundary profile reveals that it assumes stable inclinations dependent on the peaks in the fluctuation spectrum. Therefore, the inclination dependence low symmetry boundary has cusps in the vicinity of the symmetric tilt inclination, and the grain boundary stiffness cannot be extracted based on the original form of capillarity wave theory.

11:45 AM EE6.9/BB6.9
The Effect of Initial Microstructural Characteristics on Abnormal Grain Growth in Single-Phase Materials: A Mesoscopic Simulation Study. Dorel Moldovan[1] and Rakesh Kumar Behera[1,2]; [1]Mechanical Engineering, Louisiana State University, Baton Rouge, Louisiana; [2]Materials Science and Engineering, University of Florida, Gainesville, Florida.

A mesoscopic simulation methodology has been used to investigate the effect of the initial grain size distribution and grain boundary (GB) energies and mobilities on the development of abnormal grain growth in a single-phase polycrystalline material. The simulation approach is based on the Needleman-Rice (1980) variational formalism for dissipative processes. Our studies show that regardless of the initial grain size distribution, in the absence of anisotropy in GB properties, the system evolves by normal grain growth characterized by a uniform self-similar grain-size distribution, i.e. the presence of a few large grains in the initial microstructure does not promote abnormal grain growth. On the contrary, the presence of a limited set of grains having GBs with higher mobilities and lower energies may lead to abnormal grain growth provided the biased GB mobility/energy values are larger/lower than certain threshold values. Kinetic and topological aspects of normal to abnormal grain growth transition are investigated.

SESSION EE7: Time-Dependent Processes, Polymers and Composites Across the Length Scales
Chairs: John Balk and Wolfgang Windl
Thursday Afternoon, March 31, 2005
Room 2018 (Moscone West)

1:30 PM *EE7.1
Diffusion-Limited Processes Treated with Accelerated Molecular Dynamics. Murray S. Daw, Department of Physics and Astronomy, Clemson University, Clemson, South Carolina.

We treat diffusion-limited processes using Accelerated Molecular Dynamics. On-the-fly kinetic Monte Carlo is combined with the Dimer Method to find the saddlepoints exiting a valley, based on energetics from the Embedded Atom Method. With this technique, we treat two cases involving diffusion-limited processes in situations with very low symmetry. First, we calculate the tracer diffusivities in a strongly ordered intermetallic as a function of composition and temperature. Second, we treat the motion of an anti-phase boundary (APB) in the same intermetallic. We demonstrate how an APB can be moved perpendicular to itself perpendicular to itself via vacancy motion. We conclude that the on-the-fly kMC is useful over most of the range but does have "blind spots" at certain temperatures and compositions where the time boost is not sufficiently significant. The author acknowledges support from NASA (Aeropropulsion Base Research and Technology).

2:00 PM EE7.2
The Mobility and Cross-Slip of Screw Dislocations in Cu - A Molecular Dynamics Study. Dan Mordehai[1], Guy Makov[2] and Itzhak Kelson[1]; [1]Tel Aviv University, Tel Aviv, Israel; [2]Department of Physics, NRCN, Be'er Sheva, Israel.

The dynamic properties of dislocations constitute one of the basic building blocks of any theory of plasticity. One of the methodologies to study plasticity is the bottom-up approach, in which rules for dislocations kinematics and dynamics serve mesoscopic simulations. Experiments are not able yet to follow in detail the microscopic dynamic properties of the dislocation, such as dislocation motion or cross-slip, while atomistic simulations may serve as a powerful tool. Using molecular dynamics (MD) methods the dynamic properties of screw dislocations had been studied in detail for Cu, both as a function of the temperature and the applied stress. Upon applying a glide stress on the dislocation a transition from inertial to viscous motion with a stress dependent terminal velocity is observed. The experimentally observed stress dependence of the terminal velocity is reproduced quantitatively by our results [1]. If a narrow dipole of two opposite screw dislocations is introduced into the computational cell then effectively a stress is applied on the cross-slip plane. Then we observed dislocation cross slip and dipole annihilation. Upon applying a narrowing stress on the dislocation the cross-slip rate increased. From these calculations the cross-slip mechanism was identified, and the activation energy and volume were calculated as a function of model parameters, such as dislocation length and dipole width. The MD results allow us to define a set of rules for dislocation kinematics and dynamics. These rules can be used as a basic for a mesoscopic calculation. References: 1. D. Mordehai et. al. Phys. Rev. B, 67 024112 (2003) 2. http://niva.tau.ac.il/

2:15 PM EE7.3
Multiscale Elastic Relaxation in Kinetic Monte Carlo via a Lanczos Technique. Robert E. Rudd[1], Daniel R. Mason[2] and Adrian P. Sutton[3]; [1]Lawrence Livermore Natl Lab, Livermore, California; [2]Dept. of Materials, Oxford Unversity, Oxford, United Kingdom; [3]Dept. of Physics, Imperial College, London, United Kingdom.

Elastic relaxation can make significant contributions to the morphological changes observed during microstructural evolution. A technologically important case is the formation of Guinier-Preston (GP) zones, the nanoscale copper platelet inclusions responsible for the hardening of aluminum in widespread use. These metastable particles are a few atoms thick, and up to 50 nm in diameter, length scales best suited for atomistic simulation such as a kinetic Monte Carlo approach; however, previously the cost of calculating the elastic relaxation ruled out simulations sufficiently long to observe the proposed vacancy-mediated diffusion process leading to the formation of the GP zones. The elastic energy of the entire system is a principal factor determining the formation of GP zones and their evolution during aging. Here we introduce a Lanczos method to calculate the elastic relaxation that is inherently multiscale in nature and speeds up the calculation of the relaxation sufficiently to allow observation of the Cu segregation process. We present the results of these stochastic simulations. [1] D.R. Mason, R.E. Rudd & A.P. Sutton, J. Phys.: Condens. Matter 16, S2679 (2004). [2] D.R. Mason, R.E. Rudd & A.P. Sutton, Computer Physics Comm. 160, 140 (2004). Acknowledgment: This work was performed in part under the auspices of the US Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48. These simulations were performed at the Oxford University Supercomputing Centre.

2:30 PM EE7.4
A Linking Length Scale Model in Thin Film Delamination. Yueguang Wei, Haifeng Zhao and Di Jiang; Institute of Mechanics, Chinese Academy of Sciences, Beijing, Beijing, China.

A multi-scale model by which both the continuum description and the discrete dislocation description for ductile thin film delamination are linked is presented. In the continuum method for thin film delamination, the strain gradient plasticity theory is used to describe several failure processes by adopting a elastic core model, such as the interfacial fracture toughness, the shielding effects of plastic deformation on the interface crack growth, as well as the interface delaminating interface crack tip field, etc. The mechanics field around the interface crack tip by using the strain gradient plasticity theory is equivalently connected with a small scale yield solution and the stress singularity index is obtained within the strain gradient dominated region. In the microscopic delaminating analysis, the discrete dislocation theory is used to describe the shielding effects of the discrete dislocations on the interface crack growth. The result of the macroscopic analysis near the interface crack tip, i.e. a new equivalent K-field, is taken as the outer boundary condition for the microscopic delaminating analysis. The limit equilibrium locations of the discrete dislocations around the failure surfaces and the shielding effects of the discrete dislocations on the interface crack growth at micro-scale are calculated. The continuum analysis for the delaminating process and the discrete dislocation analysis for the delaminating process are linked by using the elastic core model. Through comparing both shielding effects of the plastic deformation and the discrete dislocations, the elastic core size is determined and a complete, microscopic/macroscopic delaminating process is characterized by the linking scale model. Furthermore, a ductile thin film peeling experimental result will be presented and compared with theoretical model predictions.

2:45 PM EE7.5
Multi-scale Real-Space Characterization of Layered Silicate Nanocomposites. Benji Maruyama[1], Lawrence F. Drummy[2], Hilmar Koerner[3], Ashley Tan[4], Kevin A. Heitfeld[5], Dale W. Schaefer[5], Richard A. Vaia[2] and Jonathan E. Spowart[6]; [1]MLBC, Air Force Research Laboratory, WPAFB, Ohio; [2]MLBP, Air Force Research Laboratory, WPAFB, Ohio; [3]University of Dayton Research Institute, Dayton, Ohio; [4]SOCHE, Dayton, Ohio; [5]University of Cincinnati,

Cincinnati, Ohio; [6]UES, Inc., Dayton, Ohio.

Good dispersion of the reinforcement phase in nanocomposites is recognized as critical to achieving material property goals. Hierarchical nanocomposite morphologies can be quantified by a combination of 1) Reciprocal space methods such as scattering, 2) Real space imaging such as AFM and TEM, and/or 3) Inference from established structure-property models. However, none of these techniques alone has proven satisfactory to quantitatively characterize nanocomposite morphologies across multiple length scales and link them to properties. Nor have they been adequate to define quality control metrics for dispersion. The current effort is devoted to characterizing dispersion in layered silicate nanocomposites from the nano- to meso-scales (i.e., 10 nm to 10 mm) using TEM and the Multi-Scale Analysis of Area Fractions (MSAAF) technique of Spowart et al. The MSAAF technique uses a quilting fractal analysis of real space images to generate a homogeneous length scale (scale at which the statistical variability in concentration is at some threshold), and a fractional dimension characteristic of the dispersion over a wide range of length scales. This work is part of a larger effort to determine structure/property relations of complex materials systems such as nanocomposites, and to develop representations of hierarchical morphologies as input to property models that more accurately reflect the complex nature of nanocomposites.

3:30 PM EE7.6
A Representative Volume Element Based Micromechanical Constitutive Modeling of Woven Composites.
Arunachalam M. Rajendran[1], R. Valisetty[2], R. Namburu[3] and Y. Bahei-El-Din[4]; [1]Engineering, U.S. Army Research Office, Research Triangle Park, North Carolina; [2]U.S. Army Research Laboratory, Aberdeen, Maryland; [3]U.S. Army Research Laboratory, Aberdeen, Maryland; [4]Rensselaer Polytechnic Institute, Troy, New York.

The dynamic response of woven composites under shock and impact loading is extremely complex and is greatly influenced by both geometric and material nonlinearities. For instance, the experimentally measured stress-strain responses of S-2 glass fiber based woven polyester composites under quasi-static and high strain rate loading conditions were found to be mostly linear. However, under shock and impact loading conditions, the response becomes nonlinear due to dynamic damage processes, such as matrix cracking, interfacial sliding, and fiber damage in different orientations, which could occur simultaneously and over small spatial and temporal scales. Length scales associated with the microstructure will greatly influence the local fields. The local stress and strain fields associated with these phenomena are difficult, if not impossible, to obtain experimentally. Hence, accurate, predictive analytical tools are needed to provide insights into the underlying physical mechanisms pertaining to damage. This paper presents a micromechanical material model for 3D-woven composites exhibiting progressive damage. The model is derived from actual microstructures, which possess periodic placement of the fibers in the warp, the weft and the z-directions. Local damage mechanisms that are typically found in woven systems under quasi-static and dynamic loads are modeled using a transformation field analysis (TFA) scheme. This scheme explicitly models the micro-architecture of the woven composite so that the geometric effects on local stresses and strains could be accurately computed. This modeling scheme offers a reliable approach to estimate the microscopic fields and capture the effects of the material heterogeneity and damage on wave dispersion and attenuation in shockwave problems. The TFA-based constitutive model was implemented into the DYNA finite element code and simulations of shock and impact problems were performed to describe the various damage mechanisms. The TFA model is computationally intensive and require massively parallel computing.

3:45 PM EE7.7
A Model for Predicting the Ultimate Strength of Styrene-diene Thermoplastic Elastomers based on the Failure Processes at the Molecular Level.
Qiumei Zeng and Jeremy W. Leggoe; Chemical Engineering Department, Texas Tech University, Lubbock, Texas.

Styrenic thermoplastic elastomers (TPEs) are class of triblock copolymers in which polystyrene end-blocks are combined with a variety of elastomeric polydiene midblocks. Incompatibility between the blocks results in the formation of a phase-separated microstructure, in which the polystyrene end-blocks form glassy domains (with size about 20 nm) dispersed within the elastomer matrix. The physical cross-linking provided by the hard domains enables these materials to achieve properties comparable to those of conventional vulcanized elastomers. This suggests that the PS domains play a critical role in determining the ultimate strength of these materials, though the apparently contradictory results reported in the literature indicate that a variety of other parameters must contribute to the failure process in this class of materials. The objective of this investigation has been to formulate a tensile strength model that takes into account the failure processes occurring at the molecular level in order to understand the reported variations in styrenic TPE ultimate strength. To support the development of the model, conventional and repeated loading tensile tests have been undertaken. Repeated loading tests indicate that for materials forming a cylindrical PS domain morphology, damage accumulates progressively via the break-up of the PS domains. Tensile tests over a range of strain rates determined that the ultimate strength of these materials was strongly influenced by strain rate, the ultimate strength varying by up to an order of magnitude as the strain rate increased. At the molecular level, styrenic TPEs may fail via either chain pull-out, where the PS end-blocks pull out of the glassy PS domains, or chain scission, in which the C-C bonds in the elastomer mid-blocks are ruptured. A failure model has been constructed based on determining the maximum force that can be supported by an individual chain without activating either of these fracture mechanisms; the ultimate strength is then given by the product of the maximum force and the number of activated chains crossing a cross-section. The model has been used to investigate the effect of PS content, PS molecular weight, strain rate and impurities on the ultimate strength. The model successfully predicts the trends observed in experiment.

4:00 PM EE7.8
Coupled Structural Changes at Different Length Scales Caused by Mechanical Deformation of SEBS Triblock Copolymers.
Kishore K. Indukuri, Edward T. Atkins and Alan J. Lesser; Department of Polymer Science and Engineering, University of Massachusetts, Amherst, Massachusetts.

Kraton® Triblock copolymers, consisting of two glassy-like atactic polystyrene (PS) domains coupled together by a poly (ethylene/butylene) (PE/B) flexible chain segment, have been studied using simultaneous small- and wide-angle X-ray diffraction (SAXD/WAXD) as a function of mechanical deformation in uniaxial tension. The unstrained samples have the appropriate apportioned volume fractions to self-assemble into the well established hexagonal block copolymer textural phase, i.e., where PS domains coalesce into cylindrical rods that in turn are sited on a two-dimensional hexagonal lattice within the PE/B matrix. The changes in SAXD/WAXD diffraction patterns of three different triblock copolymer compositions, with similar starting hexagonal morphologies but with systematic alterations in mid-block (ratio of ethylene to butylene segments, additional random styrene incorporation in the mid-block), were investigated. SAXD studies on unstrained samples not only show a series of concentric diffraction rings, that index as the successive orders of a two-dimensional hexagonal lattice of side a≈30 nm, but also indicate the presence of a broader, more diffuse, diffraction ring of a different character centered at a spacing of 7.8 nm. At 65% strain, a four-point X-cross pattern develops and emerges from the {10—*gravei*—0} diffraction ring for the unstrained sample. The fundamental spacing of the hexagonal lattice increases, and in addition the first evidence of discrete layer lines appears, orthogonal to the strain direction (SD). At higher strains, both the layer line spacing and the angle of the X-cross, relative to the SD, increase. These changes in layer line spacing as a function of strain provide additional insight into the extent of deformation imposed on the flexible matrix with shearing of PS cylinders layers relative to each other. Also, with increasing strain, the diffuse 7.8 nm diffraction signal transforms into a streak, parallel to the SD and centered on a reciprocal plane orthogonal to the SD. In the simultaneously recorded WAXD (4 nm-0.2 nm) patterns, an initial single diffraction ring observed at no strain, steadily transforms with strain into a symmetric pair of concentrated arcs centered on the equator. The differences in the behavior of three different triblock systems become particularly apparent in the WAXD data. These X-ray diffraction results enable a delineation to be made between rotation and relative shear of layers of PS rods and the strain-induced orientation/crystallization of the flexible matrix. Thus, these simultaneous SAXD/WAXD results provide valuable information on both the overall nature of the deformation and the coupling of specific deformation-induced structural changes at different length scales. The results also offer an explanation for the differences in the stress relaxation and the elastic hysteresis at different temperatures as a consequence of systematic alterations of the mid-block stereochemistry in these systems.

4:15 PM EE7.9
Relationship between Microstructure and Mechanical Properties of Semi Crystalline Polymers.
Fahmi Bedoui[1,2], Julie Diani[2] and Gilles Regnier[1]; [1]Laboratoire de Transformation et Veillissement des Polymeres (LTVP), ENSAM, Paris, France; [2]Laboratoire de Microstructure et Mecanique des Materiaux (LM3 - CNRS UPRESA 8006), ENSAM, Paris, France.

During the part forming, the stretching or the shearing of the polymer melt under strong cooling conditions lead to a flow-induced

crystallization, which generates specific crystalline morphologies such as deformed spherulites, shishkebab or more complex crystalline macrostructure. These crystalline microstructures generate anisotropic mechanical properties. Our interest in this work is the study of the spherulitic microstructure and its influence on the macroscopic behavior of the semi crystalline polymer. The aim of this work is to establish a correlation between the microstructure and the macroscopic behavior of these materials. To reach this aim an experimental and a micromechanical modeling protocol had been followed. The first is consisting on the investigation of the microstructure the second is to work out the elastic properties using the microstructure parameters as input. Experiments were held to investigate the microstructure of such materials. A radius spherulite gradient is observed regarding the thickness of the specimens using permanganic etching, microtome, optical and electronic microscopes. These four techniques allowed us first to quantify the radius of the spherulites and second to estimate the shape ratios of the crystalline lamellae. Also the variation of the crystallinity versus the spherulites diameter is worked out using a densimetry technique. Tensile testing were been held to correlate the microstructure properties to the mechanical properties (Young modulus). This had been reached using a removal layer technique approved in our laboratory (LTVP). This experimental approach leads us to assess enough material parameter useful in the micromechanical modeling: volume fraction of crystalline phase, morphology of the material and the shape ratios of the crystalline lamellae. The micromechanical modeling step is consisting on the estimation of the mechanical properties of the homogenized material knowing the properties of the two constituent (amorphous and crystalline phase). A differential scheme matrix/inclusion model has been successfully compared to experiment values in previous work [1]. It has been proved that given an isotropic material, the evolution of the Young modulus is governed by the crystalline fraction only. Both experiments and mechanical modeling reveal that spherulite radius change does not affect lamella shape factors as intuition could suggest. [1] F. Bedoui, J. Diani, G. Regnier; Micromechanical modelling of elastic properties in polyolefin's Polymer 2004 , Volume 45, P 2433-2442.