

SYMPOSIUM P

Nanoscale Materials and Modeling–Relations Among Processing, Microstructure, and Mechanical Properties

April 13 - 16, 2004

Chairs

Amit Misra

Materials Science & Technology Division
Los Alamos National Laboratory
MST-8, MS G755
Los Alamos, NM 87545
505-667-9860

Peter Anderson

Dept. of Materials Science & Engineering
Ohio State University
Columbus, OH 43210-1179
614-292-0176

Robert E. Rudd

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

Timothy Foecke

National Inst of Standards and Tech
MS 8553
100 Bureau Dr.
Gaithersburg, MD 20899
301-975-6592

Symposium Support

†Hysitron, Inc.
National Science Foundation
†2004 Spring Exhibitor

Proceedings to be published in both book form and online
(see *ONLINE PUBLICATIONS* at www.mrs.org)
as volume 821
of the Materials Research Society
Symposium Proceedings Series.

* Invited paper

8:30 AM *P1.1

Modeling Strength and Plasticity in Thin Films and Multilayers. William D. Nix and Bruce M. Clemens; Materials Science and Engineering, Stanford University, Stanford, California.

For passivated thin metal films and for multilayers, plasticity is controlled by dislocation flow within the crystalline layers themselves and not by diffusional wedges and the associated nucleation and glide of dislocations in the plane of the film. For such passivated films a simple kinematic strain hardening law, as suggested by Suresh, together with a temperature dependent elastic modulus, provides a good phenomenological account of plastic flow. Using this modeling approach it is possible to draw a distinction between the yield strength of the film and the strain-dependent flow stress. Models of multiple misfit dislocation formation, developed separately by Willis and Freund, are used to rationalize the linear kinematic hardening laws used in this phenomenological modeling. Applications of the Willis-Freund model to plastic deformation and strengthening of Al-Al3Sc multilayers will also be described. Plastic deformation of Al/Al3Sc multilayers is shown to be controlled by the motion of dislocations in the inherently soft aluminum layers and by the cutting of the Al3Sc layers, through the formation of antiphase boundaries.

9:00 AM *P1.2

Diffusional creep in thin films on substrates: theory, experiment and simulation. Markus J Buehler, Alexander Hartmaier and Huajian Gao; Gao, Max Planck Institute for Metals Research, Stuttgart, Germany.

In recent study of diffusional creep in polycrystalline thin films deposited on substrates, we have discovered a new class of defects called the grain boundary diffusion wedges. These diffusion wedges are formed by stress driven mass transport between the free surface of the film and the grain boundaries during the process of substrate-constrained grain boundary diffusion. The mathematical modelling involves solution to integro-differential equations representing a strong coupling between elasticity and diffusion. We show that the solution can be decomposed into diffusional eigenmodes reminiscent of crack-like opening displacement along the grain boundary which leads to a singular stress field at the root of the grain boundary. We find that the theoretical analysis successfully explains the difference between the mechanical behaviors of passivated and unpassivated copper films during thermal cycling on a Si substrate. An important implication of our theoretical analysis is that dislocations with Burgers vector parallel to the interface can be nucleated at the root of the grain boundary. This is a new dislocation mechanism in thin films which contrasts to the well known Mathews-Freund-Nix mechanism of threading dislocation propagation. Recent TEM experiments at the Max Planck Institute have shown that, while threading dislocations dominate in passivated metal films, parallel glide dislocations begin to dominate in unpassivated copper films with thickness below 400 nm. This is fully consistent with our theoretical predictions. We have developed, for the first time, large scale molecular dynamics simulations of grain boundary diffusion wedge to clarify the nucleation mechanisms of parallel dislocation in thin films. Such atomic scale simulations of thin film diffusion not only show results which are fully consistent with both continuum theoretical and experimental studies, but also revealed the atomic processes of dislocation nucleation, climb, glide and storage in grain boundaries. The study should have far reaching implications for modeling of deformation and diffusion in other micro- and nanostructured materials.

9:30 AM P1.3

Stress Generation in Amorphous Thin Films: Capillarity, Roughening, and Nanovoid Formation. Jerrold A. Floro¹, Steven C Seel¹, Paul G Kotula¹ and David J Srolovitz²; ¹Surface and Interface Sciences, Sandia National Labs, Albuquerque, New Mexico; ²Princeton Materials Institute, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey.

Real-time measurements of substrate curvature during physical vapor deposition of thin film amorphous Si, amorphous Ge, and their alloys, reveals behavior very similar to that observed during deposition of polycrystalline metal films. As a function of film thickness, a tensile regime is first observed due to island coalescence, followed by a compressive regime associated with surface stress effects, and finally by a new tensile regime associated with a surface roughening transition that leads to additional coalescence processes. These surface coalescence processes also lead naturally to nanovoid formation within the bulk of the film. Identification of the origins of these stress regimes

is aided by the lack of epitaxial strain inheritance in amorphous films, which helps decouple the thickness-dependent behavior. We will discuss the correlation of additional tensile stress generation with the internal microstructure when the amorphous films are annealed to temperatures both above and below the crystallization temperature. The effect of atomic or molecular hydrogen dosing during film growth on the surface roughness, nanovoid content, and residual stress will also be shown. This work was supported in part by the Division of Materials Science and Engineering, Office of Science, U.S. Department of Energy. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-ACO4-94AL85000.

9:45 AM P1.4

Morphological Stability of Multilayer Systems.

Sridhar Narayanaswamy¹, Peter Anderson², Amit Misra³ and Brian Cox¹; ¹Materials Division, Rockwell Scientific, Thousand Oaks, CA, California; ²Department of Materials Science, Ohio State University, Columbus, Ohio; ³MST, Los Alamos National Lab, Los Alamos, New Mexico.

Multilayer systems exhibit excellent high temperature stability when the constituent layers are immiscible and form low energy coherent interfaces. However, at elevated temperatures, if the constituent layers are miscible, rapid interdiffusion results in loss of the compositionally modulated structure and consequently, the high hardness. Immiscible layers, on the other hand, involve combinations that are thermodynamically stable with respect to each other and typically, have different crystal structures. Morphological stability issues arise even when the individual layers are thermodynamically stable. For instance, vapor-deposited immiscible multi-layers, whether coherent or incoherent, typically have columnar grain microstructures. In such polycrystalline multi-layers, thermal grooving at columnar grain boundaries crossing nanolayer interfaces influence the stability of the layered structure. The key to retaining high strengths at elevated temperatures in multi-layered materials is the morphological stability of the layered structure. With microstructural scale models, we examine the morphological stability and the kinetics of structural evolution for a multilayer system taking into account the different thermodynamic driving forces including chemical, elastic and interfacial energies. The description embodies the required conservation laws, the grain-size, physical and chemical properties of the individual layers, and flaw information to model the temporal evolution. We identify stability maps and estimate the system lifetime given the microstructural length scales and physical properties of the constituent layers and operating conditions including high temperature creep and thermal cycling.

10:30 AM *P1.5

Effects of Size on the Stiffness and Strength of Metallic Thin Films and Multilayers. Frans Spaepen, Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts.

Measurements of the modulus, yield strength and ductility of the metallic thin films and multilayers are reviewed, with special attention to the smallest length scale, down to the atomic dimension of the amorphous state. Recent data from ultra-thin metal films on polymeric substrates are included. A modulus deficit of about 0.2 is often observed in static measurements on thin films. Interestingly, a similar difference is observed between the shear moduli of amorphous metals and those of their crystalline counterparts. Mechanisms underlying this deficit are discussed, with special attention to anelastic effects revealed by stress relaxation experiments. Reports of softening with decreasing microstructural length scale ("reverse Hall-Petch") are critically reviewed. Strengthening mechanisms are reviewed, with special attention to possible contributions from strain-gradient plasticity.

11:00 AM P1.6

A new Synchrotron-Based Technique for Measuring Isothermal Stresses in Ultrathin Metallic Films.

Jochen Boehm¹, Patric Gruber¹, Ralph Spolenak², Alexander Wanner³ and Eduard Arzt^{1,2}; ¹Institut fuer Metallkunde, Universitaet Stuttgart, Stuttgart, Germany; ²Max-Planck-Institut fuer Metallforschung, Stuttgart, Germany; ³Institut fuer Werkstoffkunde I, Universitaet Karlsruhe (TH), Karlsruhe, Germany.

Most investigations of size effects on the mechanical properties of thin metallic films are based on thermal cycling experiments. However, it is favorable to decouple the changes in temperature and stress in order to better understand the fundamental mechanisms. This can be achieved by combining isothermal mechanical tests with X-ray diffraction measurements, which has been shown by several authors. Here we present a novel synchrotron-based X-ray diffraction technique, with which it is possible to characterize the evolution of stresses in polycrystalline metallic films thinner than 100 nm. We describe an experimental setup at the synchrotron X-ray source

ANKA (Karlsruhe, Germany) for monitoring the stress evolution during *in situ* tensile tests on ultrathin <111> fiber textured metallic films deposited on polymeric substrates. A strain resolution significantly better than 10^{-4} can be achieved with this technique. The samples are typically subjected to 6 % total strain and subsequently unloaded. The relative values of the principal stresses σ_1 and σ_2 depend on the elastic and plastic properties of both film and substrate. Since the complete equibiaxial stress tensor is obtained, it is possible to determine parameters relevant to plasticity such as the yield stress, the von Mises stress, the hydrostatic stress, or the triaxiality. First experiments carried out on Au films in the thickness range between 20 and 1000 nm show the usefulness and the power of this new technique. Our results show that above 300 nm, the yield strength scales inversely with the film thickness. Below 300 nm, a significant deviation from this common trend was observed.

11:15 AM P1.7

X-ray Microdiffraction Studies of Local Stresses in Thin Au Wedges, Lines and Cuboids. Ralph Spolenak¹, Mark A. Phillips¹, Nobumichi Tamura², Alastair A. MacDowell², R. S. Celestre², H. A. Padmore², B. W. Batterman^{2,3}, Eduard Arzt¹ and J. R. Patel^{2,4}, ¹Max Planck Institute for Metals Research, Stuttgart, Germany; ²Advanced Light Source, LBNL, Berkeley, California; ³SSRL/SLAC, Stanford University, Stanford, California; ⁴Dept. Materials Science & Engineering, Stanford University, Stanford, California.

The plastic behavior of small metallic structures at room temperature is determined by the interaction of dislocations with interfaces such as free surfaces and grain boundaries, and with defects such as other dislocations. TEM studies have shown the presence of dislocations in thin films even below 100 nm in thickness. In this study we present local stress measurements of Au wedges and lines which have been machined from Au thin films of 400 and 1000 nm thickness on Si substrates. The geometrical shapes were defined by using a focused ion beam to remove material from the Au films. The geometry of the wedge allows for the measurement of stress in volume elements that have roughly 100 nm as one side length. Stress was introduced by thermal cycling to 425 °C and measured in temperature steps of 50 °C. Stress measurements were performed using Laue X-ray microdiffraction with a lateral spot-size of less than one micron. As our technique also determines the density of geometrically necessary dislocations, correlations between stress-state, defect-density and interfaces (grain boundaries and free surfaces) could be observed. Grain boundaries and triple points were found to be sites of high stresses and high defect densities. The room temperature stresses in the wedge structures were also found to increase with decreasing wedge width.

11:30 AM P1.8

Tailoring Nanolaminate ALD Films for Dynamic Toughness. Neville Moody¹, John Jungk², Tom Buchheit³, Tom Mayer³, Rikard Wind⁴, Steven George⁴ and William Gerberich², ¹Sandia National Laboratories, Livermore, California; ²University of Minnesota, Minneapolis, Minnesota; ³Sandia National Laboratories, Albuquerque, California; ⁴University of Colorado, Boulder, Colorado.

Strength, friction, and wear are dominant factors in the performance and reliability of materials and devices fabricated using microsystem technologies. While adequate for some applications, as-fabricated strength and wear properties severely restrict use of these devices in many dynamic applications. Applying coatings and films is one method to enhance device performance and reliability. Atomic Layer Deposition (ALD) is ideally suited for this application as it creates conformal, stress free, and well-adhered films. Of particular interest are ALD tungsten and alumina films. However, studies on single layer ALD tungsten films showed they exhibit a pronounced susceptibility to spallation while single layer ALD alumina films exhibit lower properties than desired. We have therefore begun a study of ALD tungsten/alumina nanolaminates to determine if properties could be tailored to meet microdevice needs. The films were deposited in four, eight, and sixteen bi-layer systems to form 200 nm thick films on sapphire substrates. Nanoindentation and nanoscratch techniques using Berkovich and conical indenters were then employed to evaluate the strength, friction and adhesion of each film system at small loads characteristic of microsystem operation. These tests showed that the modulus and hardness varied slightly between systems whereas resistance to delamination and spallation varied markedly, with the four bi-layer system exhibiting the best resistance to spallation. These results will be discussed in terms of how composition, structure, and layer thickness affect adhesion and fracture susceptibility. This work supported by U.S. DOE Contract DE-AC04-94AL85000.

11:45 AM P1.9

Elastic Modulus of Nanocrystalline Niobium Thin Films. Rajarshi Banerjee¹, Evan Sperling¹, Sangita Bose², Pushan Ayyub² and Hamish L Fraser¹; ¹Materials Science and Engineering, The Ohio

State University, Columbus, Ohio; ²Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai, Maharashtra, India.

Nanocrystalline thin films of Nb with crystallite sizes varying from 5 nm to 30 nm have been deposited using high pressure magnetron sputtering under UHV conditions. The structure of these films as a function of grain size has been characterized using x-ray diffraction and TEM. With increasing pressure of the sputtering gas, there is a decrease in the average crystallite size in these films. The decrease in crystallite size in turn is accompanied by a lattice expansion in the bcc phase of Nb. There is however no evidence of a change in crystal structure with decreasing crystallite size. Nanoindentation experiments conducted on these films suggest that for crystallite sizes greater than 6 nm, there is a reduction in the modulus of these films with decreasing crystallite size. This decrease in modulus has been successfully modeled using an equation of state for metals based on the lattice expansion of the bcc Nb phase. However, for crystallite sizes less than 6 nm, there is an anomalous increase in the modulus of the thin films despite the substantially expanded lattice of the bcc Nb phase. Interestingly, independent investigations of the transport properties of these nanocrystalline Nb films suggest that at around the same critical crystallite size (6 nm), there is a metal to non-metal transition. These results and their possible implications on the elastic modulus of the Nb films will be discussed in this paper.

SESSION P2: Nanoscale Films, Dots and Multilayers – II

Chairs: Neville Moody and Cynthia A. Volkert
Tuesday Afternoon, April 13, 2004
Room 3002 (Moscone West)

1:30 PM *P2.1

Constitutive Modeling from the Bottom Up for Mechanical Behavior. William Warren Gerberich, Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN., Minnesota.

One of the major problems in assessing modeling efforts of nanolayered or nanocrystalline composites is how to choose the correct constitutive model. This can be said of almost any modeling for length scales beyond a few thousand atoms where ab initio molecular dynamics simulations currently become impossible. Some density functional theory approaches handle much larger numbers but then the potential choice is often problematic without real property checks and balances. On the experimental side it is the establishment of small volume constitutive behavior that has been elusive. The convergence of these bottom up theoretical and top down experimental approaches is being made possible by STM, AFM and nanoindentation scanning probe techniques. We report on two major findings, one of Si and Ti nanospheres and the other of Au nanoboxes. In the silicon case, new results on nanosphere compacts evaluated under high pressure will be compared to individual nanosphere properties. In a parallel study, 200 nm Au nanoboxes with a wall thickness to height ratio of about 0.12 are compared to solid Au thin films of the same 200 nm thickness, the latter being grown on sapphire. While little connectivity to atomistic simulations is possible at this juncture, some interesting length scale issues associated with scale-up problems will be highlighted. Specifically, it will be demonstrated that surface energy effects, dislocation nucleation and image force considerations, and state of stress effects must all play a major role in constitutive modeling at the nanoscale. While some of these are automatically handled by atomistic scale simulations, others will have to be included in larger scale mesoscopic systems which include discretized dislocations.

2:00 PM P2.2

Mechanical Properties of Nanoporous Au. Cynthia A. Volkert¹, Ruth Schwaiger², Thorsten Dietz¹, Dominik Kramer¹, Joerg Weissmueller¹ and Oliver Kraft¹; ¹Forschungszentrum Karlsruhe, Karlsruhe, Germany; ²MIT, Cambridge, Massachusetts.

The mechanical properties of nanoporous materials are of interest because of their potential application as hydrogen storage and actuator materials and because of possible dramatic size effects due to the nanometer scale dimensions of the pores and cell walls. In order to investigate their mechanical properties, a recently developed method for performing uniaxial compression tests on micron sized specimens [1] has been applied. Following this method, a Focused Ion Beam microscope was used to cut columns with diameters between 0.1 and 6 μm and heights between 1 and 10 μm from single grains in the sample surface. The columns were then compression-tested using a nanoindentation system. Initial results have been obtained from nanoporous Au samples with a nominal relative density of 40% and pores and cell wall sizes of roughly 20 nm. The Young's modulus obtained during unloading of the columns was roughly 12 GPa, which

is in excellent agreement with the expected value for idealized porous Au of this density [2]. Clear evidence for plasticity and/or brittle crushing set in at stresses of around 100 MPa and increased to stresses as large as 300 MPa at a total strain of roughly 35%. Based on purely geometrical scaling laws, plastic collapse or brittle crushing of the nanoporous Au would be expected at 3 and 36 MPa, respectively. The very much larger stresses measured here are a clear indication of a tremendous increase in both the yield and fracture strengths of the cell wall material, presumably because of the small dimensions. Careful microscopy after testing revealed that non-porous columns had deformed by localized slip, while the porous columns were homogeneously compressed. The strain applied to the nanoporous columns was accommodated by uniform lateral expansion of the column and only a small fraction (10%) of the applied strain contributed to densification. The apparent linear work hardening (5% of elastic modulus) is thus presumably due to an increase in the stress required for plastic deformation or fracture of the cell walls. Tests are underway to investigate the mechanical behavior and the deformation morphology as a function of the crystal orientation, column dimensions, strain rate, and pore size. [1] M.D. Uchic, D.M. Dimiduk, J.N. Florando, and W.D. Nix, *Mat. Res. Soc. Proc. Vol 753 BB1.4.1* (2002). [2] L.J. Gibson and M.F. Ashby, "Cellular Solids: Structure and Properties", Pergamon Press (1988).

2:15 PM P2.3

Nanomechanical Imaging and Nanoscale Elastic Modulus Measurements from SN Nanobelts. Yuegui Zheng¹, Pulickel Ajayan² and Robert E. Geer¹; ¹School of Nanosciences, University at Albany, Albany, New York; ²Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, New York.

Self-assembling nanoscale materials have long been investigated for their unique mechanical, electrical, optical, or biological properties. Regarding the former, however, direct measurement of the nanomechanical properties of self-assembled nanoscale structures has long been hampered by the lack of appropriate nondestructive methodologies. Recently, the self-assembly of Sn-based 'nanobelts' synthesized via chemical vapor deposition has been reported. These systems possess rectangular cross-sections. Widths range from 20 nm to 1 micron. Cross-sectional aspect ratios range between 0.5 and 1. Here we present the first direct nanomechanical imaging and nanoscale modulus measurements of such systems. Sn-based nanobelts ranging in width from 200 nm to 1 micron were studied. Electron diffraction measurements revealed the nanobelts considered here possessed a single-crystal diffraction pattern indicating an a-Sn FCC structure with the (110) axis parallel to the nanobelt surface normal. Subsequent atomic force microscopy (topography) revealed atomically smooth surface features with the exception of 'nano-dot' domains with a radius of 70 nm and a height of 4 nm. The latter showed faceting implying crystalline registration with the underlying crystalline structure of the nanobelt. Coupled with the TEM data we preliminarily conclude the nano-dots consist of nucleated domains of Sn. Nanomechanical imaging was undertaken via ultrasonic force microscopy (UFM) to investigate the variation of the surface mechanical compliance. A uniform mechanical response was exhibited by the smooth regions of the nanobelt as well as the nano-dot regions. Differential-UFM was used for quantitative measurement of the local contact stiffness. This technique investigates the pico-indentation of a the ultrasonically vibrating belt against an inertially-damped AFM tip. The probed region consisted of a 10nm x 10nm area. The nanobelt modulus was estimated at 25 GPa using the SiO₂ substrate as a calibration standard. The nano-dots exhibited the same modulus. These measurements reveal lower elastic moduli than expected from bulk measurements.

2:30 PM P2.4

Evaluation of Interface Strength between Copper Submicron Dot and Silicondioxide Substrate. Hiroyuki Hirakata, Takayuki Kitamura and Yoshitake Yamamoto; Department of Engineering Physics and Mechanics, Kyoto University, Kyoto, Japan.

An experimental method for evaluating interface strength of a submicron dot on a substrate is developed using a modified Atomic Force Microscopy (AFM), which can control and measure precisely the load and the displacement of the tip. This technique is applied to copper (Cu) cylindrical dots of submicron scale (diameter: 300 nm 800 nm, height: 50 nm) on a silicondioxide (SiO₂) substrate. A hard tungsten (W) layer is introduced over the top surface of the Cu dot to restrain the fracture and the plastic deformation of the dot. A loading tip is positioned at the surface of the SiO₂ substrate near the dot at first, and it is dragged horizontally along the SiO₂ surface under a constant displacement rate. The lateral as well as the normal load and displacement of the tip are continuously monitored during the test by means of the modified AFM. After the tip hits the W layer the lateral load increases almost proportionally with the lateral displacement. The Cu dot then is abruptly separated from the substrate along the interface without nonlinearity in the load-displacement relation. No

damages are observed near the tip-contacted region of the W layer. The maximum load required to separate the interface increases with the diameter of the dot. A finite element analysis reveals that the concentration of shear stress occurs near the Cu/SiO₂ interface edge where the interface crack is initiated. The interface strength is evaluated by the concentrated stress.

2:45 PM P2.5

Utilizing on-chip testing and electron microscopy to obtain a mechanistic understanding of fatigue and wear in polysilicon structural films. Daan Hein Alsem^{1,2,3}, Eric A. Stach^{2,3}, Christopher L. Muhlstein⁴, Michael T. Dugger⁵ and Robert O. Ritchie^{1,2}; ¹Materials Science and Engineering, University of California, Berkeley, Berkeley, California; ²Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California; ³National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, California; ⁴Materials Science and Engineering, Pennsylvania State University, University Park, Pennsylvania; ⁵Materials and Process Science Center, Sandia National Laboratory, Albuquerque, New Mexico.

Wear and fatigue are important factors in determining the reliability of microelectromechanical systems (MEMS). While the reliability of MEMS has received extensive attention, the physical mechanisms responsible for these failure modes have yet to be conclusively determined. In our work, we use a combination of on-chip testing methodologies and electron microscopy observations to investigate these mechanisms. Our previous studies have shown that fatigue in polysilicon structural thin films is a result of a 'reaction-layer' process, whereby high stresses induce a room-temperature mechanical thickening of the native oxide, which subsequently undergoes environmentally-assisted cracking. In this presentation, we discuss how the initial native oxide thickness affects the fatigue life positively and report on new *in vacuo* observations. This allows us to characterize both the changes in fatigue behavior and the development of reaction layers in a relatively oxygen-free environment. Additionally, we have used polysilicon MEMS side-wall friction test specimens to study active mechanisms in sliding wear at the microscale, including the role of the surface conditions. In particular, we have performed *in vacuo* and *in situ* experiments in the scanning electron microscope, with the objective of determining the mechanisms causing both wear development and debris generation.

3:30 PM *P2.6

Strength Limits for Thin Cu and Au Films Approaching the Nanoscale. T. John Balk, Linda Sauter, Gerhard Dehm and Eduard Arzt; Max-Planck-Institut fuer Metallforschung, Stuttgart, Germany.

As their thickness and grain size decrease toward the nanoscale, thin films exhibit less plasticity during thermal cycling. Eventually, threading dislocations are no longer able to be generated within the confinement of the thin film geometry, due to the prohibitively high stresses required. In unpassivated Cu, the deformation mechanism switches to parallel glide for films thinner than 400 nm, and film strength ceases to increase with decreasing film thickness. In this case, virtually all of the plastic deformation in the film is accommodated at the grain boundaries via constrained diffusional creep. As grain size reaches 100 nm, however, a single dislocation mediates the necessary plasticity and parallel glide dislocations are no longer emitted from the grain boundaries. For both passivated and unpassivated thin metal films, we have observed strength plateaus in the nanoregime. For unpassivated copper and gold, the flow stress measured at the end of thermal cycling is constant for films between 400 and 35 nm. The plateau value corresponds to approximately $\mu/240$ for both metals, indicating that this apparent limit of strength is far below the theoretical shear strength. Additionally, Cu films passivated with 10 nm of oxidized aluminum also appear to exhibit a plateau in strength, albeit starting at a film thickness of 100 nm. For passivated Cu, the maximum strength is approximately 1400 MPa and corresponds to $\mu/110$, also significantly less than the theoretical shear strength. These apparent plateaus and trends in the thickness dependence of flow stress will be explained in light of observations obtained during thermal cycling of thin films in the transmission electron microscope.

4:00 PM P2.7

Size Effect on Crack Formation in Ta/Cu and Ta/Cu/Ta Thin Film Systems. Patric Gruber¹, Jochen Boehm¹, Ralph Spolenak², Alexander Wanner³ and Eduard Arzt^{1,2}; ¹Institut fuer Metallkunde, Universitaet Stuttgart, Stuttgart, Germany; ²Max-Planck-Institut fuer Metallforschung, Stuttgart, Germany; ³Institut fuer Werkstoffkunde I, Universitaet Karlsruhe (TH), Karlsruhe, Germany.

Many efforts have been made to investigate size effects on the mechanical properties of thin metallic films on the nanoscale. Most of these investigations have been based on thermal cycling experiments. In doing so Balk et al. observed a new deformation mechanism responsible for a plateau flow stress was observed for Cu films thinner

than 300 nm. This so called parallel glide mechanism is caused by constrained diffusional creep, which involves diffusion between the unpassivated film surface and the grain boundaries at elevated temperatures. In order to investigate the influence of temperature and Ta passivation and interlayers on this mechanism, we applied a recently published novel synchrotron X-ray diffraction technique to characterize the evolution of isothermal mechanical stresses during in situ tensile tests in ultrathin polycrystalline Cu films. The film systems were deposited by magnetron sputtering under UHV conditions on polymeric substrates. The Ta film thickness was always 10 nm, whereas the Cu film thickness varied between 20 and 3000 nm. All samples were subjected to 6 % total strain and subsequently unloaded. In addition to influencing the diffusive processes, the Ta layers produced different effects on the deformation behavior of the film systems. Samples with a Cu film thickness below 300 nm showed a sudden stress decrease at a total strain of about 2.5 %. This was attributed to fracture of the entire film system caused by cracks in the Ta layers. Above 300 nm Cu thickness, we assume that cracking in the Ta layers was compensated by plastic flow within the Cu layers. The unpassivated Ta/Cu films exhibit an apparent plateau in yield strength, which is attributed to cracking in the Ta interlayer, rather than to constrained diffusional creep.

4:15 PM P2.8

Structure-Property Relationships of Au Films Electrodeposited on Ni. Chris San Marchi¹, Neville R Moody¹, Megan J Cordill³, Gene Lucadamo¹, James J Kelly¹, Thomas Headley² and Nancy Yang¹, ¹Sandia National Laboratories, Livermore, California; ²Sandia National Laboratories, Albuquerque, New Mexico; ³University of Minnesota, Minneapolis, Minnesota.

Thin gold films and coatings on metal have long constituted an important technology for the microelectronics industry and will continue to be important for microdevices such as contact springs. The properties of these materials may be highly processing dependent, particularly when the gold is deposited by electrochemical means. In this study, we characterize 1 μ m thick gold electrodeposited on Ni substrates from two bath chemistries, gold sulfite with hardening additive and gold cyanide. TEM and SEM show that the bath chemistry alters the microstructure and the resulting surface of the electrodeposits. Nanoindentation techniques were then used to determine the elastic and plastic properties of the various gold coatings. Hard gold films produced from the sulfite bath have grain sizes as small as 20 nm, in some cases substantial twinning, and fine porosity uniformly distributed both within the grains and at grain boundaries. The hardness is about 2 GPa, approaching the hardest values reported for sputtered gold films. We, thus, compare the characteristics of our electrodeposited gold to gold films deposited by sputtering and evaporation. In addition, AFM is used to identify indicative deformation mechanisms in these electrodeposited gold films.

4:30 PM P2.9

Nanoscale Structure and Electronic Transport Correlations in Cu-Nb Bilayers*. Michael Hundley¹, Ana Lima¹, Amit Misra¹, Xinghang Zhang¹, Eric Bauer¹ and Corwin Booth², ¹Los Alamos National Laboratory, Los Alamos, New Mexico; ²Lawrence Berkeley National Laboratory, Berkeley, California.

We examine the interplay between nanoscale structures and macroscopic materials properties by investigating the anomalous temperature-dependent resistivity exhibited by a series of nanometer length-scale Cu-Nb bilayer films. Measurements of the temperature-dependent dc electrical resistivity and Hall effect are reported in the temperature range 4 K to 450 K. The bilayer films were prepared by dc magnetron sputtering onto a variety of substrates including Si(100), Si(111), MgO, GaAs, glass, Al₂O₃, and kapton. The thickness of both elemental layers is equivalent in all film studied, and the total film thickness was varied from 0.5 μ m to 5 μ m. For individual layer thickness ranging from 1 to 5 nm the dc resistivity exhibits very large, hysteresis-free anomalies that occur at a substrate, repeat-length, and film-thickness dependent temperature. Depending on the specific sample parameters this characteristic anomaly temperature can range from below 100 K to near 400 K. The temperature-dependent resistivity is characterized by a high-temperature state of anomalously low resistance and a low-temperature state of high resistance. In comparison, films with repeat lengths greater than roughly 10 nm exhibit a monotonic, nearly temperature-independent resistivity that is comparable to the low-T resistivity exhibited by the thinner films. By comparing the data to bilayer transport models it appears that the transport anomalies may stem from strain-induced variations in carrier scattering at interfaces and grain boundaries. We use cross-sectional transmission electron microscopy and local-structure measurements to correlate the transport properties with nanoscale film structures. *work performed under the auspices of the US Department of Energy

4:45 PM P2.10

Modeling the Elastic Fields in Epitaxially grown Multilayers. Ganesh Vanamu¹, Tariq A Khraishi², Abhaya K Dartye¹ and Saleem H Zaidi³, ¹Chemical and nuclear, University of New Mexico, Albuquerque, New Mexico; ²Mechanical Engineering, University of New Mexico, Albuquerque, New Mexico; ³Gratings, Inc., Albuquerque, New Mexico.

We have calculated strain energy density for three and four layers of graded Ge (SixGe1-x) on silicon. A model was developed to calculate the elastic fields in multilayers grown epitaxially on a planar substrate. This model works well for compliant and non-compliant substrates. Using the equations for static equilibrium and Hooke's law for isotropic materials under a plane stress condition, the elastic fields associated with each layer were calculated. The strain partitioning in this model reduces to the limiting case of a two-layer structure. Strain partitioning is a function of the bulk unstrained lattice parameters, elastic constants and thicknesses of the layers. The model was qualitatively verified by comparing the strain energy density with the dislocation density away from a relatively thick substrate. This model helps in growing defect free multilayers for optoelectronic devices.

SESSION P3: Poster Session: Nanoscale Films, Particles and composites
Tuesday Evening, April 13, 2004
8:00 PM
Salons 8-9 (Marriott)

P3.1

Effect of Mold on the Temperature Distribution of Sintered Body in the Plasma Activated Sintering. Gil-Geun Lee, Div. of Materials Science and Engineering, Pukyong National University, Busan, South Korea.

Recently, the plasma activated sintering process has been used for preparing various nanostructured materials. Maintenance of homogeneous temperature distribution in the sintered body during plasma activated sintering was very important for obtaining functional nanostructured materials. In the present study, the focus is on the effect of dimension of mold on the temperature distribution of sintered body during plasma activated sintering. Ten kinds of cylindrical molds have various dimensions of length, inner diameter and outer diameter were prepared using graphite. The change of the temperature distribution in the mold with mold dimension was measured using thermocouple and pyrometer. The temperature distribution was changed by the change of the mold dimension. The effect of the inner diameter and outer diameter of the mold on the change of temperature distribution was higher than the one of the mold length. The temperature homogeneity of sintered body was depended on a relative ratio of the dimension function of the mold.

P3.2

Determination of Ion Irradiation Influence on π -plasmon Properties of Carbon Nanotubes. Mariya M. Brzhezinskaya¹, Eugen M. Baitinger¹ and Vladimir V. Shnitov², ¹Physics, Cheliabinsk State Pedagogical University, Cheliabinsk, Russian Federation; ²Ioffe Physical-Technical Institute, Saint Petersburg, Russian Federation.

Modifications of ion irradiation of carbon nanotubes lead to changes in nanotubes structure. Varying the chemical composition of the flow, the energy and the irradiation dose allows to generate defects in structure and to weld and curve carbon nanotubes. The degree of the ion irradiation influence on the nanotubes has to be determined during the process and upon its completion. Energy electron loss spectroscopy represents one of the effective methods for determining the degree of influence since it measures plasmon properties, which are very sensitive to a degree of defects and orderliness of the carbon nanotubes. The MWNTs were 8 \pm 16 nm in diameter and approximately 10 μ m in length. The MWNTs were periodically irradiated by argon ions with energy of 1 keV. The doses of Ar⁺ irradiation varied from 36 to 360 μ C/cm². The loss spectra of reflected electrons were measured at several different energies of primary electrons in the region from 100 to 1500 eV (error was 0.5 eV). The analyzer operated in the mode of constant absolute energy resolution $\Delta E = 0.6$ eV. Operating vacuum was not worse than 5 \cdot 10⁻⁹ Torr. Results indicate the π -plasmon energy E_{π} and the full width at half maximum (FWHM) of the plasma peak were sensitive to the dose of ion irradiation. In particular, the π -plasmon energy E_{π} decreases ($\Delta E_{\pi} = 1.2$ eV) and the plasma peak widens with the increase of the dose of Ar⁺ irradiation. The accuracy of determination of plasmon energy was 0.11 eV. The π -plasmon peak widening is associated with a result of MWNTs damage under ion irradiation. Possible causes of the carbon nanotubes deformation and its influence at π -band structure of carbon nanotubes are discussed.

P3.3

The Role of Al in Mechanical Alloyed Ti-Al-B Nanocomposite by Spark Plasma Sintering (SPS). Young Hwan Han² and Hyung

Bock Lee¹; ¹Inorganic Materials Engineering, Myong-Ji University, Yongin, South Korea; ²Chemical Engineering and Materials Science, University of California, Davis, Davis, California.

Ti-Al-B composite was successfully consolidated by SPS with the activated nano powders by Mechanical Alloying, which were just before complete synthesis stage, and TiB₂ crystalline particles with 10-30 nm and Al with unreacted Ti and B on the grain boundaries exist as a ternary phase. Three different Al compositions doped with the reactively formed TiB₂ during Mechanical Alloying played a critical role on consolidation and mechanical property. The nanocomposite of Ti-Al-B system was consolidated by SPS and characterized on microstructure and mechanical property, which was synthesized from activated nano powders by Mechanical Alloying. Planetary ball milling was used for Mechanical Alloying for 120-180 min with 350 rpm. The synthesized activated powders were pressed at 1400°C under 60 MPa in vacuum, with 1800 A(DC) for 4 min. The synthesized Ti-Al-B nanocomposite was analyzed by SEM, XRD and TEM, with a TiB₂ second phase in 10-30 nm size, and remained amorphous phase of Al with unreacted Ti and B on grain boundaries as a ternary phase. In the composition of 0.3 mol Al, the relative density of 98% and bending strength of 847 MPa were higher than those of TiB₂ composite, and the hardness measurement of 19.6 GPa in the 0.1 mol Al.

P3.4

First-Principles and ab initio Molecular Dynamics Studies on Energetics and Kinetics for Electro-Active Polymers: PVDF and P(VDF-TrFE). Haibin Su¹, Alejandro Strachan² and William A. Goddard III¹; ¹Materials and Process Simulation Center, Caltech, Pasadena, California; ²Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico.

We use a combination of density functional theory with the generalized gradient approximation (DFT-GGA) and a first principles-based force field (denoted MSXX FF) with molecular dynamics (MD) to study static and dynamical mechanical properties of the ferroelectric polymer Poly(vinylidene fluoride) (PVDF) and its copolymer with trifluoro ethylene (TrFE). We use DFT-GGA to calculate structures and energetics for various crystalline phases for PVDF and P(VDF-TrFE). For PVDF the lowest energy phase is non-polar with a combination of trans and Gauche bonds, the role of the bulkier F atoms in the copolymer is to stabilize Trans conformations; this leads to a higher crystallinity and piezoelectricity observed experimentally. Using the MSXX FF we calculate domain wall energies as well as the nucleation energy necessary to form a Gauch bond in an all-Trans crystal. We find a much lower energy for the P(VDF-TrFE) copolymer (14.9 kcal/mol) than for PVDF (24.8 kcal/mol), this correlates with the fact the polar phase of the copolymer (denoted I) exhibits a solid-solid a transition to a non-polar phase under heating while PVDF directly melts. We have also studied the mobility of an interface between a polar and a non polar phase as a function of the applied tensile stress. We find a smaller threshold value of stress and higher mobility in the case of the copolymer. Finally, we characterized the process of plastic deformation under shear deformation for P(VDF-TrFE); our simulations show that chains find very low resistance to sliding, particular along the chain direction. We show that atomistic simulations can reveal important information regarding the fundamental mechanisms that govern the electromechanical behavior of this important class of materials, such a molecular understanding may provide valuable guidelines for materials design.

P3.5

Nanocalorimetry Study of Glass Transition of Ultra Thin Polymers. Mikhail Yu. Efremov, Eric A. Olson, Ming Zhang, Zishu Zhang and Leslie H. Allen; Department of Materials Science and Engineering and Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois.

The thermophysical properties of ultra-thin polymer coatings are the subject of strong interest due to experimental, technological and theoretical issues regarding size-dependent effects [1]. Glass transition in ultra-thin (1 - 400 nm thick) spin-cast polymer films of polystyrene, poly (2-vinyl) pyridine and poly (methyl methacrylate) is investigated by the ultra-sensitive differential scanning calorimetry technique ("nanocalorimetry") [2]. Using this method, the glass transition in selected polymers can be observed even at thickness as low as 1-3 nm [3]. The glass transition temperature is assigned using the concept of limiting fictive temperature. We do not find a noticeable dependence of the glass transition temperature on thickness in films ranging between several hundred nanometers down to 3 nm thick [3]. Effects of broadening of transition dynamics and loss of transition contrast will be discussed. Literature [1]. J. A. Forrest, Eur. Phys. J. E 8, 261

(2002). [2]. M. Yu. Efremov, E. A. Olson, M. Zhang, F. Schiettekatte, Z. S. Zhang, and L. H. Allen, Rev. Sci. Instr., in press. [3]. M. Yu. Efremov, E. A. Olson, M. Zhang, Z. Zhang, and L. H. Allen, Phys. Rev. Lett., 91, 085703 (2003).

P3.6

Prediction of Melting Temperature of Nanoclusters by Atomistic Simulations. Ho-Seok Nam¹, Nong M. Hwang², B. D. Yu³ and D.-Y. Kim¹; ¹Center for Microstructure Science of Materials, School of Materials Science and Engineering, Seoul National University, Seoul, South Korea; ²School of Materials Science and Engineering, Seoul National University, Seoul, South Korea; ³Department of Physics, University of Seoul, Seoul, South Korea.

The calculation of the melting temperature of materials is of fundamental interest, representing a fundamental understanding of the equilibrium properties of system. The melting line may be determined directly if we know the Gibbs free energy of both solid and liquid phases as a function of temperature and pressure. The difficulty in the application of this simple thermodynamic principle to nanocluster is that the free energy of system cannot be trivially calculated. On the other hand, in conventional molecular dynamics simulations, the melting temperature of nanoclusters can be estimated from the caloric curve by measuring the total potential energy of system with the slow increase of temperature. However, due to the limitation of simulation time scale in molecular dynamics, this method does not guarantee thermodynamics equilibrium in spite of granting that the superheating of solid cluster is negligibly small. Therefore, we introduce an alternative way of determining the melting temperature using umbrella-sampling method combined with constrained molecular dynamics simulation. In this method, we can obtain the Landau free energy curves near the estimated melting temperatures and determine the melting point by interpolating the relative free energy difference between the solid and liquid phases. In this research, the melting point of 459-atom Au nanocluster was predicted based on the semi-empirical embedded-atom method. Additionally, the particular melting behavior of Au nanoclusters reported by molecular dynamics simulations [Phys. Rev. Lett. 81, 2036 (1998)] could be explained well by the calculated free energy curves.

P3.7

Testing Multiwall Carbon Nanotubes on Ion Erosion for Advanced Space Propulsion. Yoke Khin Yap¹, Jitendra Menda¹, Lakshman Kumar Vanga¹, Vijaya Kayastha¹, Jiesheng Wang¹, Lyon B King², Svetlana Dimovski³ and Yury Gogotsi³; ¹Physics, Michigan Technological University, Houghton, Michigan; ²Mechanical Engineering-Engineering Mechanics, Michigan Technological University, Houghton, Michigan; ³Materials Science and Engineering, A. J. Drexel Nanotechnology Institute, Drexel University, Philadelphia, Pennsylvania.

Are carbon nanotubes more resistant than diamonds against ion erosion? Here, we report the evaluation of multiwall carbon nanotubes (MWNTs) as the protective coating against plasma erosion in advance space propulsion systems. The space exploration program faces enormous challenges as it seeks to achieve dramatic improvements in safety, cost, and speed of missions to the frontiers of space. Plasma propulsion systems have been recognized as far more efficient than chemical thrusters. This recognition has led to the development of highly efficient electric propulsion (EP) thrusters that are currently the only feasible technology for many deep space missions. However, these EP devices have in common electrode sputter erosion as a life-limiting process. To facilitate long thruster life, critical surfaces in EP thrusters are fabricated from sputter-resistant materials such as molybdenum (Mo). Carbon-based materials have shown nearly an order-of-magnitude improvement in sputter erosion resistance over Mo. Among the tested carbon-based materials, CVD diamond films provide improvement by a factor of 1.5 in volumetric sputter erosion rate over others. Unique mechanical properties of carbon nanotubes have triggered tremendous curiosities on their applications. We have tested MWNTs for ion erosion and compared them to CVD diamond films, boron nitride (BN), and amorphous-carbon (a-C) films. Two types of MWNTs were used. First, MWNTs were grown vertically aligned to the substrate surface by a dual-RF-plasma enhanced CVD system. Secondly, MWNTs were grown by thermal CVD so that their tube axes are aligned parallel to the substrate surface. All BN and a-C films are grown by our pulsed-laser deposition (PLD) system. All these samples were placed directly in the exhaust beam of a flight-quality 1.35-kW Hall-effect thruster. Each sample was partially masked such that a portion of the material was exposed to ion erosion, while a portion was protected. The thruster was operated on krypton propellant with a discharge voltage of 300 V and a current of 1.8 A. Post-test analyses of the samples included scanning electron microscopy (SEM) images taken at the masked and the exposed areas, profilometry across the masking boundary in an attempt to determine the eroded depth, Raman spectroscopy etc.. Our results indicate that only CVD diamond films and vertically aligned MWNTs survived the

ion erosion. Furthermore, formation of vertically aligned MWNTs bundles was discovered in these experiments. The formation of these bundles, the erosion mechanism of MWNTs, and the comparison between MWNTs and CVD diamond films will be discussed in the paper. These results show that vertically aligned MWNTs are promising for application in EP thrusters of advanced space propulsion systems.

P3.8

PET/Mesoporous Material Nanocomposites: the Novel Pattern of Polymer/Inorganic Composites. qu ling¹, Tong Da ming², Xiao yong zhuang² and Dou Tao²; ¹Shanghai Research Institute of Petrochemical Technology, Shanghai, China; ²Taiyuan University of Technology, Taiyuan, China.

Polymer/layered silicate nanocomposites have attracted much attention as the properties of polymers are much superior to that of the corresponding unfilled and conventionally-filled micro-composites counterparts. Based on this pattern, in this paper we reported the first engraftment of porous silicate mesoporous materials as the inorganic fillers on poly (ethyleneterephthalate) to prepare the PET/MCM-41 nanocomposites by direct PET polymer melt penetration. Utilizing the pore engineering technique we expanded the pore size of MCM-41 to provide the large pore space for the melted PET molecular chains to penetrate the pores easily. The structure and morphology of the nanocomposite were determined by X-ray diffraction and scanning electron microscopy techniques. The XRD diffraction of the PET/MCM-41 sample exhibited no characteristic peaks of MCM-41, demonstrating that the amorphous and weak pore walls of MCM-41 were exfoliated after the incorporation of PET. SEM images of PET/5%MCM-41 nanocomposite also showed the formation of exfoliated particles of pore wall in the nanocomposite. DSC measurement indicated that the nanocomposites have a higher crystallization rate than that of pure PET due to the nucleating effect of the exfoliated pore wall particulate as well as possess the higher heat of crystallization (55.4J/g) and corresponding the higher relative crystallinity (49%) which compared with other inorganic nucleating agents of PET, which perfectly solve the well-known contradiction of the increased crystallization rate with the decreased crystallinity existed for conventional fillers.

P3.9

The effect of shear forces on microstructure and mechanical property of epoxy/clay nanocomposite. Tak-Keun Oh, Ajit Bhaskar, Charles Beatty and Hassan El-Shall; Material Sci & Eng, University of Florida, Gainesville, Florida.

The objective of this work is to understand the shear force effect on the preparation of epoxy-clay nanocomposites. The commercial organoclay (Cloisite 30B) was used in this research. The shear force was controlled with changing RPM (revolutions per minutes) on the mechanical mixer. It was found that differences in the aspect ratio of clay layers and differences of clay particle distribution in the epoxy matrix by shear force. X-ray, TEM and SEM investigated the degree of exfoliation and morphology. The mechanical and thermal properties were also studied. This study revealed that appropriate shear force and mixing time on the nanocomposite preparation was required to achieve the ultimate properties.

P3.10

Computer Simulated 3D Virtual Reality for Dynamical Modeling and Calculations of Carbon-Based Nanocomposites. Maksim V Kireitseu, ¹Composite materials research laboratory, University of New Orleans, New Orleans, Louisiana; ²Mechanics and Composites, Institute of mechanics and machine reliability, Minsk, Belarus.

The principal goal of the paper is to reveal at what scale principal Newtons fundamentals may give reliable explanations at examining fracture mechanics and rheological behavior of carbon-based fullerene-like nanostructures. Pure interfaces diamond-like C / metal structure (matrix) was studied. Diamond nanoparticles have spherical, fullerene or pyramidal-type shapes and carbon-based nanotubes and fibers as well. Local structure deformation (rearrangement) of diamonds/metal interfaces was principal object of researches. Energy or band structure and density of electronic states analysis was investigated. Possible defect or surface states were described. The core of principal Newtons fundamentals was combined with rheological modeling for describing correlation between stress and deformation of nanostructured coatings. Rheological modeling and finite elements technique as methods for determining the fracture of nanocomposites are described. The task of this paper was to present the modified linear augmented Slater-type orbital method (LASTO) for solving Schrodinger's equation in nanodiamonds crystals with arbitrary atoms per unit cell. It follows to expect this method will allow more efficiently calculating an electronic band structure and structural energy difference for vary transition nanocomposites. As a result

overlap matrix and hamiltonian matrix elements were derived in details. The relativistic generalization of the linear augmented Slater-type orbital method (RLASTO) for solving Dirac's equation in diamonds nanoparticles crystals with arbitrary atoms per unit cell was also described. It follows to expect this method will allow more efficiently calculating an electronic band structure and structural energy difference for vary transition metal compounds taking account all necessary relativistic effects. As a result overlap matrix and Hamiltonian matrix elements were derived. We offer an application of modern software engineering tools (nanoCAD, CAM, CASE) for modeling virtual reality and molecular dynamics of novel nanocomposites. The main components of presented system are 1) software and nanoengineering tools for modeling of virtual reality, molecular dynamic of novel diamonds-containing nanocomposites. Recent advances in computer modelling and simulations of the mechanics of materials at the nano and micro scales are reviewed. The Multiscale Modeling of Materials (MMM) approach is shown to rely on systematic reduction of the degrees of freedom at natural length scales. Connections between such scales are currently achieved either by a parameterization or a coarse graining procedure. Parameters that describe the system at a lower length scale are obtained from computer simulations, often verified experimentally, and passed on to upper scales. Alternatively, lower length scale descriptions can be coarse-grained through a zoom-out process.

P3.11

Preparation, Characterization and Mechanical Properties of Epoxidized Soybean Oil/Clay Nanocomposites. Zengshe Liu¹, Sevim Erhan¹ and Jingyuan Xu²; ¹FIO, NCAUR, USDA/ARS, Peoria, Illinois; ²CPF, NCAUR, USDA/ARS, Peoria, Illinois.

In recent years the interest in nanoscale materials was inspired by the fact that nanoscale materials often exhibited physical and chemical properties that were dramatically different from their bulk counterparts. One of the most promising composite systems would be organic polymers and inorganic clay minerals consisting of silicate layers. The polymers prepared from readily available renewable resources have become increasingly important. The advantages of these polymers are their low cost, mostly biodegradable and environmentally friendly. Among products from agricultural resources, natural oils may constitute raw materials useful in polymer synthesis. In this study we report the preparation, characterization and mechanical properties of epoxidized soybean oil (ESO)/clay nanocomposites. X-ray diffraction (XRD) measurements and transmission electron microscopy (TEM) were taken for the characterization of formed nanocomposites. We also performed viscoelastic property measurement to get storage modulus (G') and glass transition temperature of these materials. Tensile test was performed to study how of the presence of nanofillers alters the mechanical properties of nanocomposites.

P3.12

Characterization of the Mechanical and Fracture Behavior of Epoxy Phenolic Nanocomposites. Maria Lujan Auad¹, Steve Nutt¹ and Patricia M. Frontini²; ¹MCGILL Center for Composite Materials - Materials Science, University of Southern California, Los Angeles, California; ²Materials Science Department, INTEMA, University of Mar del Plata, Argentina, Mar del Plata, Argentina.

Nanocomposites of modified montmorillonite clays in a glassy epoxy-phenolic were prepared. Relationship between the chemical network structures and the physical properties of the epoxy-phenolic nanocomposite has been elucidated. The thermal and mechanical properties were measured and it was found that compared to the matrix, the nanocomposites exhibited far greater improvement in properties over the neat matrix for a given silicate fraction. The increase in the mechanical performance was correlated with the network properties. The results were consistent with most particulate-filled systems. The fracture toughness of these materials was investigated and improvements in toughness values of 60% over unmodified resin were demonstrated. SEM micrographs were taken from fracture surfaces of net and nanocomposites materials to further understand the fracture mechanism.

P3.13

Debonding Under Fatigue Loading of Polymer/Inorganic Interfaces. Bree Sharratt¹ and Reinhold H Dauskardt²; ¹Aeronautics and Astronautics, Stanford University, Stanford, California; ²Materials Science and Engineering, Stanford University, Stanford, California.

The effects of cyclic fatigue loads on subcritical debonding of a polymer layer from an adjacent substrate are of significant interest for the integrity of components used in applications ranging from automotive sensors to high density electronic packages. However, limited experimental studies have been conducted in the area of accelerated interfacial crack propagation under alternating fatigue

loads. In addition, the associated micromechanisms of cycle-by cycle damage accumulation and fatigue crack growth in the interfacial region between the highly constrained polymer and adjacent elastic substrate are largely unknown. In this presentation, we examine such interfacial fatigue crack growth at the interface between a model polymer system and two inorganic dielectric substrates (Si_3N_4 , SiO_2) under Mode I loading. The effects of fatigue loading history and loading ratio are presented. Comparisons of interfacial crack growth rates with those produced under monotonic loading are made with particular emphasis on the near threshold crack growth behavior. High resolution characterization of the resulting fatigue crack surfaces revealed the surprising presence of fatigue striations which are used to propose a mechanism for the observed fatigue behavior.

P3.14

Abstract Withdrawn

P3.15

Influence of Deposition Rate on the Crystallization Kinetics and Surface Microstructure of Amorphous Nb₂O₅ Thin Films. Rand David Dannenberg and Eric A Stach; Rockwell Scientific, Thousand Oaks, California.

As the deposition rate increases in a thin film process, adatom burial of the growing film impedes surface diffusion, and the grain size can decrease from the millimeter scale through the nanoscale, to the amorphous state. In this scale, it is known that mechanical properties vary rapidly with small changes in grain size. Nb₂O₅ is an important high index of refraction dielectric material used commonly in thin film optical filters. Using in-situ heating stage TEM, we report on the influence of the deposition rate on the kinetic variables describing the crystallization process: activation energy; velocity pre-exponential. Surface roughness is also correlated to scattering losses in transmitted light. We comment on this materials use in optical filters where the index of refraction is varied over nanometer length scales, and the modeling of the optical behavior of such systems.

P3.16

The Manufacturing & Impact Response of Carbon/Epoxy Composites Reinforced with SiC Nano Particles.

Nathaniel Chisholm, Hassan Mahfuz, Renee' Rodgers, Vijaya Rangari and Shaik Jeelani; T-CAM, Tuskegee University, Tuskegee, Alabama.

Room temperature cure epoxy resin has been doped with SiC nanoparticles through an ultrasonic cavitation process. The modified resin is then utilized in a Vacuum Assisted Resin Transfer Molding (VARTM) process with satin weave carbon fibers to manufacture nanophased composite panels. The nanoparticles were spherical in shape and about 29 nm in diameter. The loading of nanoparticles into the resin ranged from 1.5 to 3.0 percent by weight. The mixing of nanoparticles with Part-A SC-15 resin was carried out in a Sonic Vibra Cell ultrasonic liquid processor at 55% of the amplitude for about 30 minutes. At this time, the dispersion of nanoparticles seemed uniform through visual observation. In order to avoid rise in the temperature during sonication, cooling was employed by submerging the mixing beaker in a mixture of ice and water. Part-B (hardener) was then added with the mixture at a ratio of 3:10 and the mixing was carried out mechanically for about 10 minutes using a high speed mechanical stirrer. In the next step, the mixture was used in a VARTM setup with satin weave carbon preforms to fabricate nanophased composite panels. Once cured, test coupons were extracted and subjected to both quasi-static and dynamic loading. Under quasi-static loading tensile and flexural response were of particular interests. Dynamic tests were also carried out at low velocity impact and at high rates of strain. Details of manufacturing, analyses of mechanical tests and enhancements in properties due to nanoparticle infusion are discussed in this paper.

P3.17

Synthesis of Zeolite As Ordered Multicrystal Arrays.

Jim Seok Lee, Yun-Jo Lee, Eunju Lee Tae, Yong Soo Park and Kyung Byung Yoon; Chemistry, Sogang University, Seoul, South Korea.

Zeolites are crystalline nanoporous aluminosilicates widely used in industry. In order for zeolites to find applications as innovative materials, they need to be organized into large two- and three-dimensional (2D and 3D) arrays. We report that uniformly aligned polyurethane films can serve as templates for the synthesis of uniformly aligned 2D and possibly 3D arrays of silicalite-1 crystals, in which the orientations of the crystals are controlled by the nature of the polymers. We propose that the supramolecularly organized organic-inorganic composites that consist of the hydrolyzed organic products and the seed crystals are responsible for this phenomenon.

P3.18

Using Theory and Simulation to Design Self-Healing Nanocomposite Thin Films Jae Youn Lee, Zhenyu Shou,

Gavin Buxton and Anna C. Balazs Chemical and Petroleum Engineering Department University of Pittsburgh, Pittsburgh PA 15261. Anna C. Balazs, Chemical Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania.

Thin films that are composed of polymers and inorganic nanoparticles offer the flexibility and processability of the polymers and the mechanical, optical and electromagnetic properties of the inorganics. Thus, these composite films are vital to the fabrication of various high-performance, lightweight materials. These thin layers are, however, susceptible to crack formation, which can form within the interior or at the surface of the system. Using a hybrid computational model, we focus on thin films of polymers and nanoparticles to design materials where the nanoparticles migrate to cracks within the system and effectively form patches to repair the damaged regions. We also use a micromechanical simulation to probe the structural integrity of the repaired layers. By contrasting the properties of the system in the damaged and healed states, we can determine the effect of the nanoparticle patches. Through these studies, we can isolate optimal conditions for harnessing nanoparticles to act as responsive band-aids for composite materials and to maximize the performance of the patched interfaces.

P3.19

Synthesis and Study of Nanostructures Via Microwave Heating. Oxana Vasilievna Kharissova¹, Eder Zavala¹, Ubaldo

Mendez Ortiz², Jose Luis Pinero Hernandez³ and Stanislav Soloviev⁴; ¹Facultad de Ciencias Fisico-Matematicas, Universidad Autonoma de Nuevo Leon, San Nicolas de los Garza, Nuevo Leon, Mexico; ²Facultad de Ingenieria Mecanica y Electrica, Universidad Autonoma de Nuevo Leon, San Nicolas de los Garza, Nuevo Leon, Mexico; ³Facultad de Ciencias Biologicas, Universidad Autonoma de Nuevo Leon, San Nicolas de los Garza, Nuevo Leon, Mexico; ⁴Department of Chemistry, University of South Carolina, McAllen, South Carolina.

This work is devoted to microwave heating of graphite, sucrose, calcined sucrose, and a mixture of graphite with sucrose to produce carbon nanotubes (CNTs). The samples were submitted to microwave radiation (power 800W, frequency 2.45 GHz) in air and high vacuum (10⁻⁵ Torr) for 30 to 60 min. The oven temperature was approximately 1200 celsius degrees. After vaporization the condensed material was collected on various fused silica targets (different morphologies were used). The samples were found to contain a significant proportion of nanotubes, nanoparticles and fibers (1-2.8 micrometers), which appeared to be highly graphitized and helical structured. After deposition, the morphology of carbon nanotubes was studied with SEM, TEM and AFM techniques. It was observed that multi-walled nanotubes (MWNTs) were produced by this method. The morphology of fused silicon based substrates (quartz and silicon carbide) was studied as an important factor for the growth of carbon nanotubes. The size and shape of the obtained nanotubes on different substrates (porous and non-porous fused silicon substrates) were analysed, as well as the their concentration across the substrate and other properties.

P3.20

Fabrication and Characteristic of Zirconia and Zirconia-Alumina Composites With Bilayered Structure.

Sung-Jae Je¹, Myung-Won Lee¹, Jae-Ean Lee¹, Yeon-Gil Jung¹ and Dong-Su Park²; ¹Department of Ceramic Science and Engineering, Changwon National University, Changwon, Kyungnam, South Korea; ²Ceramic Materials Group, Korea Institute of Machinery and Materials, Changwon, Kyungnam, South Korea.

Bilayered structure with inner layer of ZrO₂-3mol% Y₂O₃ (TZ-3Y) and outer layer of zirconia-alumina (AKP-30 or synthesized Al₂O₃) composite is fabricated using gel casting for the inner layer and dip coating for the outer layer in aqueous system, respectively. We are objective to fabricate the porous substrate for damage absorption that can also improved adsorption of alumina slip or precursor sol and form zirconia-alumina composite through infiltration into the zirconia substrate. The processing additives for gel casting, such as dispersant, monomer, dimmer, and initiator, are adjusted and optimized. From which the solid loading of each starting material is determined. The optimal amount of dispersant for each starting material using the D3019 as anionic dispersant agent is 0.7 wt% for TZ-3Y and 0.5 wt% for AKP-30. The suspensions pH affects the electric double layer in sols, resulting in viscosity and solid loading of each starting material. The castable solid loading of TZ-3Y ceramic powder is 37 vol%, showing pseudoplastic rheological behavior. The effects of suspension types on sintered bodies fabricated are studied through microstructure, density, strength, and Vickers indentation. The strength of sintered bodies with dip coating into alumina slip or sol is higher than that without dip coating, but hardness is not much difference between both cases. The effects of thickness of outer layer on damage resistance and mechanical properties of the bilayered structure are discussed extensively.

P3.21

Synthesis of dual porous silica with zeolite core/mesoporous shell and corresponding rectangular carbon capsules.

Jong-Sung Yu and Suk Bon Yoon; Chemistry, Hannam University, Daejeon, South Korea.

There has been great deal of interest in creating core-shell composite materials and capsules with tailored structural, optical and surface properties using spherical nanoparticles as molds. Various procedures have been applied to fabricate uniform coated and stable colloidal particles. Herein we would like to report the fabrication of dual porous silica with ZSM-5 zeolite core/mesoporous shell by forming a uniform mesoporous shell over the respective rectangular zeolite crystal core. The carbon capsules with hollow core/mesoporous shells were also fabricated using the dual porous zeolite core/mesoporous shell silica as sacrificial templates. The resulting carbon capsules have bimodal pore systems consisting of a uniform rectangular hollow core and of a mesoporous shell with uniform thickness of 40–50 nm. The dual porous silica with zeolite core/mesoporous shell and the corresponding carbon capsules will have potential for wide range of applications including catalysts, adsorbents, sensors, electrode materials, and advanced storage materials.

P3.22

Effect of substrate bias on structure and properties of nanocomposite WC-C films prepared by a novel hybrid deposition system. Ai-Ying Wang and Kwang-Ryeol Lee; Future Technology Research Division, Korea Institute of Science and Technology, Seoul, South Korea.

Tungsten-containing diamond-like carbon films were deposited on silicon (100) wafer substrates by a hybrid process combining DC magnetron sputtering with an end-hall ion gun source. During the films deposition, a wide range of DC negative bias from 0 to 600V was applied to the substrate holder and W concentration in the films could be controlled by varying the Ar / C₆H₆ ratio of the mixed gas in the discharge chamber. The structure and properties of the films were analysed by Rutherford backscattering spectroscopy, Raman spectroscopy, stress surface profilometer, nanoindentation, TEM, and so on. It was demonstrated from the Raman spectra that the intensity ratio of D peak to G peak (I_D / I_G) for all samples had a lowest value at the bias voltage of approximately 200V, which usually represented the highest sp³ bonded carbon in the films. As a result, the highest residual stress (σ), hardness (H) and Young's modulus (Y) were all obtained at the bias voltage of 200V. Simultaneously, it was found that the residual stress in the films was significantly reduced with the increase of W concentration in the films, which showed the incorporation of nano-scale WC particles to amorphous carbon matrix played an important role in the structural and mechanical properties of the films.

P3.23

Marked Increase in the Binding Strength between the Substrate and the Covalently Attached Monolayers of Zeolite Microcrystals by Molecular Cross-Linking between the Neighboring Microcrystals. Jin Seon Park, Yun-Jo Lee and Kyung Byung Yoon; chemistry, Sogang university, seoul, South Korea.

Monolayers of cubic zeolite microcrystals (1.7 x 1.7 x 1.7 micro-m³) were assembled on glass plates through imine-linkages between the zeolite-tethered 3-aminopropyl (AP) groups and the glass-bound benzaldehyde groups, which were prepared by treating AP-tethering glass plates with a large excess of terephthalaldehyde (TPDA) in toluene. The additional treatment of the monolayers of zeolite microcrystals with TPDA led to molecular cross-linking between the neighboring, closely packed zeolite microcrystals in the monolayers through AP-TPDA-AP imine linkages between the zeolite-tethered AP groups and the newly introduced TPDA. The comparison of the binding strengths between the glass substrates and the monolayers revealed that the molecular cross-linking leads to as much as seven-fold (by average) increase in the binding strength.

P3.24

Intra-Tube Radial Elastic Modulus Measurements of Individual Carbon Nanotubes. Frederick Heuchling¹,

Yuegui Zheng¹, Pulickel Ajayan² and Robert E Geer¹; ¹School of Nanosciences, University at Albany, Albany, New York; ²Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, New York.

Carbon nanotubes represent a singular example of a molecular system offering emergent functionalities derived from its nanoscale size. It has been aggressively researched for uses in nanocomposites owing to its outstanding mechanical properties and in nanoelectronics for both its metallic and semiconducting character. Previous investigations of multi-walled carbon nanotubes (MWNTs) from this group have

demonstrated significant intra-tube variations in the relative radial modulus due to the presence of volume defects or 'necking'. To further investigate intra-tube variations of mechanical response a quantitative methodology for extraction of radial modulus from individual multi-walled carbon nanotubes has been developed. This protocol is based on so-called differential ultrasonic force microscopy (d-UFM). Here, the contact stiffness of an area on the order of 10nm x 10nm is measured directly with an atomic force microscope tip using ultrasonic vibration. This technique has been shown to be effective for materials ranging in modulus from 100 MPa to 300 GPa. MWNTs produced via high-temperature (> 850 oC) chemical vapor deposition were investigated. Transmission electron microscope imaging revealed a relatively narrow core implying a large number of concentric walls. Subsequent UFM measurements revealed a uniform mechanical compliance of the MWNT along its axis. D-UFM measurements carried out over small (10nm x 10 nm) regions of the MWNT revealed a radial modulus exceeding that of Si (> 160 GPa). The latter measurement was taken from the substrate area adjacent to the MWNT of interest. These observations agree with predictions that MWNTs with small core radii should exhibit significantly higher resistance to radial deformation compared to MWNTs with a small number of walls.

P3.25

Characterization of Carbon Nanotubes/Cu Nanocomposites Processed by Using Nano-size Cu Powders. Kyung-Tae Kim, Kyong-Ho Lee, Seung-Il Cha, Chan-Bin Mo and Soon-Hyung Hong; Materials Science and Engineering, Korea Advanced Institute of Science and Technology, Daejeon, South Korea.

Carbon nanotubes (CNTs) has been considered as an ideal reinforcement for composite materials due to its outstanding properties such as high strength, elastic modulus, aspect ratio and conductivities. However, compared to CNT/polymer and CNT/ceramic nanocomposites, the CNT/metal nanocomposites attract less attention due to their lower mechanical properties than expected. Even though several researchers have fabricated CNT/metal composites by powder metallurgy process including mixing of CNTs with metal powders and followed by hot pressing, the CNT/metal nanocomposites show low relative density ranged 85–95% and, at the same time, severe agglomeration of the CNTs in a matrix. In this study, CNT/Cu nanocomposites were fabricated by powder metallurgy process by mixing of CNTs with Cu powders and followed by spark plasma sintering of mixed powders. In order to investigate the effect of initial size of Cu powders on microstructure and mechanical properties of CNT/Cu nanocomposites, two different sizes of Cu powders such as 100nm and 200 μ m, were mixed with the CNTs. In order to obtain higher densification of CNT/Cu nanocomposites, the spark plasma sintering process was used. As a result of microstructural observation on sintered CNT/Cu nanocomposites, when the nano-sized Cu powders were used, the CNTs were homogeneously intermixed with Cu powders, while, when the macro-sized Cu powders were used, most of the CNTs were agglomerated at the surface of Cu powders. Also, the result of hardness shows a considerable enhancement in only CNT/Cu nanocomposites fabricated by using the nano-size Cu powders. The hardness increases with increasing the CNT volume fraction up to 10% and the peak hardness of 102kg/mm² was obtained for the CNTs/Cu nanocomposites, which was approximately 1.5times higher than that of unreinforced Cu consolidated using the nano-size Cu powders.

P3.26

Responsive Polydiacetylene/ Amine Nanocomposites.

Byron McCaughey¹, Xuan Li¹, Jiebin Pang¹, Xiang-Ling Ji¹, C

Jeffrey Brinker³ and Yunfeng Lu¹; ¹Chemical Engineering, Tulane University, New Orleans, Louisiana; ²Chemistry, Tulane University, New Orleans, Louisiana; ³Sandia National Laboratories, Albuquerque, New Mexico.

Nanoscale materials often show unique and superior properties due to the dimensional constraint, interfacial effects, enhanced interactions, and other nanoscale phenomena. Self-assembly techniques have emerged as one of the most efficient routes to synthesize nanoscale materials. This presentation reports the synthesis and novel properties of polydiacetylene (PDA) nanocomposites through self-assembly using diacetylene containing acids and amines as building blocks. PDA has been the subject of extensive work because of its ability to form stable, ordered thin films that change color due to thermal, mechanical, or chemical stimuli. Based on non-covalent networks of hydrogen bonding, π - π stacking, hydrophobic, and electrostatic interactions between the building blocks, PDA nanocomposites with highly ordered monoclinic crystalline structure are synthesized. These nanocomposites have been studied using FTIR, XRD, TEM, AFM, UV-vis and other techniques. The unique molecular architecture and tunable building blocks endow these novel materials with reversible thermochromatic transitions, self-healing mesostructure, preferential amine sensing and reversible intercalation. For example,

nanocomposites shows a complete thermochromatic reversibility between 25°C and 85°C even after 30 thermal cycles. Over this same temperature range, a reversible order-disorder transition due to the weak intramolecular interactions accompanies the thermochromatic response. Such self-healing and reversible thermochromatic materials are of importance for tunable optical filter, chemical sensors, pressure sensors, and other applications.

P3.27

Non-equilibrium Molecular Dynamics of Shock Induced Thermite Reaction. Vikas Tomar and Min Zhou; George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, Georgia.

Molecular dynamics (MD) simulations are an important tool for characterizing the influence of nanoscale effects which determine the energy release rate and extent of reaction in reactive metal oxide powder mixtures. This research focuses on the development of a computational framework for large-scale MD simulations of shock-induced reactions. The system under study is a Fe₂O₃+Al thermite mixture. The MD modeling involves the development of an interatomic potential for the Fe+Al+Fe₂O₃+Al₂O₃ system. A variable charge cluster functional potential for the system is developed. The model is capable of describing the multi-component behavior of the system and the qualitative energetics of the association and the dissociation during thermite reactions. The potential uses electronegativity equalization to account for changes in the charge of different species according to local environment. Parameters in the potential are determined by fitting to the properties of Fe, Al, Fe₂O₃, and Al₂O₃. In addition, NPT molecular dynamics simulations are carried out to verify the accuracy of the potential. The results show that the potential can account for the energetics of the thermite reaction. A parallel non-equilibrium molecular dynamics (NEMD) code is developed to study the shock-induced detonation behavior of the Fe₂O₃+Al system. The simulations involve various loading conditions and nano phase morphologies. It is found that the reactions are affected by a multitude of factors including phase morphology, loading rate, loading, and voids.

P3.28

Size dependence of elastic properties of LPCVD silicon nitride. Yuxing Ren, Stanley Y.Y. Leung, Jun Wang and David C.C. Lam; Mechanical Engineering Department, The Hong Kong University of Science and Technology, Kowloon, Hong Kong.

Mechanical properties of thin films such as the yield strengths and the hardnesses of metals are reported to exhibit size dependent behaviors, and the elastic moduli of thin silicon cantilever beams fabricated from SOI wafers are dependent on thickness. In this investigation, the size dependence of the elastic properties of silicon nitride thin films is investigated using nanoindentation and beam bending. A series of silicon nitride micro-cantilevers were fabricated using LPCVD. Nanoindentations on the silicon nitride revealed that the elastic properties were thickness dependent. To confirm the dependence, the elastic deflection behaviors of the beams loaded at different distances away from the anchor were characterized. Load-deflection data showed that the normalized bending rigidities, which should remain constant if the elastic properties were size independent, showed significant size dependence. The normalized beam bending rigidity decreased by more than 50% as the thickness is reduced from 730nm to 350nm. Microstructural characterization using X-ray diffraction revealed that the thick beams contained a higher fraction of crystalline phase than the thin beams. Higher normalized rigidity appeared to be associated with crystalline phase content. To confirm the hypothesis, a set of beams was annealed in a reducing environment. Depth-profiling XPS was used to characterize the samples before and after annealing and the compositions were found to be similar. X-ray diffraction data on the annealed set showed that the annealed beams contained a higher fraction of crystalline silicon nitride phase; and bending of the annealed beams revealed that the normalized bending rigidities are markedly larger than that of the un-annealed beams. The difference in the fraction of crystalline phase is identified to be the principal origin of the size dependence in elastic properties. The difference in crystalline phase fraction is suspected to be associated with CVD deposition time. On this basis, the relation between processing, microstructure and resulting mechanical properties are discussed.

P3.29

Nano-structured Ceramics Composites by Novel Casting Method from Multi-component Oxide Melts.

Masahiro Yoshimura, Shunji Araki, Jose M. Calderon-Moreno, Sophie Le Gallet, Hiromasa Suzuki and Tomoaki Watanabe; Dept of Materials Sciences and Engineering, Tokyo Institute of Technology, Yokohama, Japan.

Nano-structured ceramic composites have attracted lots of researchers and engineers. Generally, most of polycrystalline bulk ceramics have

been made from fine powders via their shape forming and sintering, not via melt/casting, because melt/solidified ceramics would crack during cooling. In order to prevent the accumulation of residual stresses, we have tried to make the samples by rapid solidification of eutectic systems. In the ternary systems of Zirconia (Hafnia)-Alumina-YAG, we have succeeded to fabricate nano-structured bulk ceramics by just simple solidification of the melt. The mixed powders were melted into a globule with 3-5 mm diameter by an arc-imaging furnace, then cooled rapidly. The spherical samples were transparent, no cracking and consisted of 20-100 nm size crystals: Zirconia (Hafnia)-Alumina-YAG. Zirconia (Hafnia)-Alumina-ABO₃ perovskite systems would give transparent amorphous phases, which can be changed into nanocrystalline bulk composites by appropriate annealing i.e. HfO₂-Al₂O₃-GdAlO₃ nano-composites have been fabricated by annealing at 1200°C or 1400°C. Those ceramic nano-composites can be applied for wide areas: structural, functional, and coating materials. 1)J.M. Calderon and M. Yoshimura, *Solid State Ionics*, 141/142, 343 (2001) 2)S. Araki and M. Yoshimura, *J. Euro. Ceram. Soc.* accepted(2003)

P3.30

Abstract Withdrawn

P3.31

Fabricating nanoscale structures with near-substrate electric field. Wei Lu and David Salac; Mechanical Engineering, University of Michigan, Ann Arbor, Michigan.

Electric field is an excellent driving force to control structures on length scales difficult to manipulate in other manner. This paper reports our work on fabricating nanoscale polymer structures with a near-substrate electric field. If is found an in-plane electric field parallel to an air-polymer interface could induce interface instability, leading to the formation of nanoscale polymer structures. The non-uniformity in the field distribution essentially limits the size and location of nanostructures. The process is simulated with the finite element method.

P3.32

Dimensionally Controlled Growth of Nano-grained Films on Chemically Self-assembled Gold Nanotemplates. Uma Chopali, Pritish Mukherjee and Sarath Witanachchi; Laboratory for Advanced Materials Science and Technology, Department of Physics, University of South Florida, Tampa, Florida.

Granular films deposited by physical vapor deposition processes typically contain a broad distribution of grain sizes in the micrometer range. The ability to grow and control the grain sizes in nanostructured films is especially important for hard coatings. In this paper we present a new technique that combines a chemical self-assembly process and a physical vapor deposition process to deposit films with uniformly distributed nanograins. The first step in this method is the use of a reverse micelle technique to form mono-dispersed gold nanoparticles as a colloidal solution. The particle size is controlled in the range of 10-100 nm by the solvent concentration. The particles are coated with the surfactant Na(AOT) to prevent agglomeration, followed by spin coating on a glass substrate, causing them to self-assemble in a 2D array. Subsequent to evaporating the volatile surfactants, the gold nanotemplate on the substrate is used as the growth surface for film deposition. A dual-laser ablation technique is used to deposit TiC and TiN films on these functionalized substrates. The morphology of the nanotemplates and the films was studied by Atomic Force Microscopy (AFM). The grain size distribution and the effect of grain size on the film hardness, studied by x-ray diffraction and nano-indentation techniques, will be presented.

P3.33

Interface studies and phase transformations in nanostructured carbide derived carbon. Sascha Jorg Welz¹, Yury Gogotsi²; Michael McNallan³; ¹Chemical Engineering and Materials Science, UC Davis, Davis, CA; ²Materials Engineering, Drexel University, Philadelphia, PA; ³Civil and Materials Engineering, University of Illinois at Chicago, Chicago, IL.

In this study, the formation mechanism of nanocrystalline diamond on metal carbides during etching in halogens at ambient pressure and moderate temperatures are analyzed. HRTEM studies of the metal carbide/diamond interface show that direct epitaxial growth of diamond on metal carbides is possible, which is in agreement with our molecular dynamics simulations. Stress may be introduced at the metal carbide / diamond interface forming dislocations due to the mismatch of the lattice parameters. Annealing of carbide derived carbon (CDC) leads to graphitization. The phase transformation process of 2H diamond to graphitic carbon onion structures is observed and can be described as zipper-like process. Carbon onions are identified as high-pressure cells and may be responsible for a high

elastic recovery of the CDC film during mechanical testing.

P3.34

Microstructures Development in Reaction Processed CoContinuous Composites. Glenn Daehn¹, Jim Nash¹, Ed Del Rio¹, Andrew Strange² and Michael Breslin²; ¹Materials Sci & Eng, Ohio State University, Columbus, Ohio; ²Excera Materials Group, Columbus, Ohio.

While more traditional discontinuously reinforced composites typically have properties that are qualitatively similar to those of the continuous phase, co-continuous or interpenetrating-phase composites have a mix of properties that is a bit harder to predict. Also these materials have seen less development and application. Co-continuous composites can often be created by various types of displacement reactions. Here we will show some of the interesting processing structure relations that are developed by the reactive infiltration of silica bearing precursors into liquid aluminum alloy melts. This develops a co-continuous alumina-aluminum composite. Typically the alumina structure that grows has a strong texture with the alumina c-axis aligned in the growth direction. Also the alumina colonies that grow are strongly oriented with each other, with 60 degree boundaries dominating the structure. The morphology of the silica precursor has an important effect, modest amounts of porosity frustrate growth reducing the strength of the texture and alignment relations. Also the alloy content of the bath plays an important role; decreasing the aluminum activity can dramatically refine the structure, bringing the characteristic dimension from microns to tens of nanometers. This kind of structural control is of clear importance in developing materials of this class for elevated temperature service.

P3.35

Mechanical Properties of DLC/Polyurethane Composite Characterized by Nano-indentation. Sang Hyun Yoon¹ and Rajiv Singh²; ¹Materials Science & Engineering, University of Florida, Gainesville, Florida; ²University of Texas, Austin, Texas.

Diamond-like carbon (DLC) films have been the subject of intensive studies for the last decade because of their unique properties such as high hardness, high wear resistance, chemical inertness, etc. Depending on the deposition system used, DLC with different contents of hydrogen and various compositions of carbon hybridizations can be produced for versatile applications. Hydrogen incorporated amorphous carbon (a-C:H) and tetrahedral carbon (ta-C) films are the two most representative forms of DLC family. In this study, electron cyclotron resonance chemical vapor deposition (ECR CVD) and pulsed laser deposition (PLD) techniques were used to fabricate these two different types of DLC films to compare their structures and properties and investigate the application feasibility of produced DLC films. Our preliminary results acquired by nano-indentation measurements of DLC coatings on Si(100) substrates showed that relatively soft ($E = 139.26$ GPa, $H = 11.56$ GPa) a-C:H films were produced from ECR CVD. On the other hand, relatively hard ($E = 187.33$ GPa, $H = 21.54$ GPa) ta-C films were produced by PLD. Therefore, coupled with the possible low temperature process, DLC/polymer composite can be fabricated to increase the mechanical properties and life time of polymer component. The nano-indentation results of these composites exhibited the unique 2-step unloading behavior, which resulted from the hetero-structure of two completely different layers. The properties of DLC coating layers can be controlled by selecting the proper deposition conditions.

P3.36

Measurements of the Internal Strain and Structural Dynamics of ZnS Nanoparticles. Benjamin Gilbert, Feng Huang, Hengzhong Zhang and Jillian F Banfield; Earth & Planetary Sciences, University of California - Berkeley, Berkeley, California.

The change in electronic properties of nanoparticles as a function of particle size can be explained in many systems by quantum confinement without recourse to descriptions that include size-dependent structural effects. However, the structure of very small particles can be profoundly different from that of the equivalent bulk material. Changes in structure can be induced by changing both particle size and the surface environment and may lead to significant modification of nanoparticle properties. Based on studies of two-dimensional surfaces of bulk materials it is anticipated that nanoparticle surfaces will be reconstructed. We are currently unable to directly characterize nanoparticle surface structure. However, strain associated with the surfaces that bound the nanoparticles can drive structural changes throughout, and these may be investigated by methods that probe real space interatomic distance distributions. Here, we apply the technique of pair distribution function (PDF) analysis to compare the structures of approximately 3 nm ZnS nanoparticles in the presence of weakly or strongly interacting surface ligands. The PDF is the real-space interatomic distance correlation function, obtained from wide-angle X-ray scattering (WAXS). In

contrast to diffraction patterns, small particle size alone does not broaden peaks in the PDF. Furthermore, interatomic correlations can be detected at considerably greater distances than is possible with extended X-ray absorption fine structure (EXAFS). For ligands such as methanol, water, and mercaptoethanol the PDF shows a crystalline core that is significantly smaller than the particle size. The intensities of longest-range (thus surface-weighted) correlations in the PDF are suppressed, indicating that reconstruction occurs and that there is little structural coherence between different areas of the nanoparticle surface. Structural disorder, seen by the diameter of the internal crystalline core, strongly decreases with increasing surface ligand strength. Nanoparticle structure can respond dynamically at room temperature to changes in surface ligand, as shown by the structural transformation associated with water-binding. We observed the structural differences between bulk ZnS and 3 nm mercaptoethanol-coated ZnS nanoparticles by making a comparison between interatomic correlation lengths of up to 15 Å. Results show that surface strain drives anisotropic contractions of interatomic distances throughout the particles. A temperature-dependent EXAFS study of lattice dynamics shows that this structure modification is associated with lattice stiffening.

P3.37

Multiscale Mechanical Studies of Nacre from the Gastropod Mollusk Trochus Niloticus. Benjamin Bruet, Hang Qi, Mary C. Boyce and Christine Ortiz; Materials Science and Engineering, MIT, Cambridge, Massachusetts.

The inner columnar nacreous layer of the gastropod mollusk *Trochus Niloticus* is a nanostructured biocomposite with outstanding and unique mechanical properties. It is composed of 95% wt of hexagonal aragonite plates (width 5 nm, thickness 0.87 nm), stacked 40 nm apart, and 5% wt of a biomacromolecular "glue" which exists between and within the individual plates. Atomic Force Microscopy (AFM) revealed a dense array of nanoasperities on the top and sides of the aragonite plates (120 nm wide, 4.6 nm high). A multiscale theoretical and experimental approach was taken to identify, understand, and predict the complex deformation mechanisms and mechanical behavior of this fascinating material. Macroscopic 3-point bend tests yielded an in-plane Young modulus of 68.0 GPa for freshly cut samples and a fracture strength of 231 MPa. Uniaxial compression yielded Young moduli of 6.4 GPa for samples with the brick layers oriented parallel to the load, 2.9 GPa when oriented perpendicular to it and fracture strengths of respectively 223 and 475 MPa. The discrepancy between the moduli emphasizes that very distinct deformation mechanisms prevail during these tests, which is confirmed by the fact that fracture occurs also in three different ways (respectively through thickness, interlaminar and burst). Scanning Electron Microscopy (SEM) and AFM of failed samples revealed jagged and branched crack fronts at plate interface, tortuous crack paths, non-uniform angles of polygons (suggesting possible intrinsic deformability and displacement/sliding). The technique of nanoindentation was carried out on individual aragonite tablets using a diamond-coated Berkovich probe tip (end-radius of 70 nm, tip angle of 142.3 degrees), at rates of indentation ranging from 1 nN/s to 100 nN/s (load controlled), forces from 10 nN to 10 mN and indentation depths from 10 to 370 nm. AFM inspection of the indented region showed the existence of extensive plastic deformation within the tablet suggesting that occluded biomacromolecules may play a significant role in the deformation. Finite element simulations are also being developed to quantitatively determine the behavior of nacre under a wide range of stress configurations at various scales. A 3D elastic-perfectly plastic model was built and the deformation of 1/6 of the indenter and material solved numerically. Comparison of the simulation results with nanoindentation data yielded an excellent fit for a modulus of 76 GPa and a yield stress of 3-4 GPa. This study shows that a biocomposite principally composed of a poor ceramic (aragonite) can achieve surprisingly good macroscopic mechanical properties thanks to a complex hierarchical structure allowing an extraordinary variety of energy-dissipating mechanisms. Our aim is to continue to formulate multiscale structure-property relationships to eventually aid in the design and advancement of new synthetic biologically inspired lightweight, hard body armor technologies.

P3.38

Simulation of Sintering of Nano-Size Silver Particles. Veena Tikare, Michael V. Braginsky, Nelson Bell and Thomas Headley; Sandia National Laboratories, Albuquerque, New Mexico.

Experimental investigation of sintering of silver nano-particles showed anomalous behavior between 300 to 350 °C. Particle connectivity decreased slightly in this temperature range. In an attempt to understand this behavior a kinetic, Monte Carlo model was used to study the connectivity of particles when the grain boundary energy and pore surface energy changed with respect to each other. The model simulates all the process contributing to solid state sintering in a simple, single phase system such as silver. It simulates curvature

driven grain growth; pore migration and pore shape equilibration by surface diffusion; and formation, grain boundary diffusion, and annihilation of vacancies. This paper applied this model to investigate the anomalous sintering behavior of silver nano-particles. We found that desintering can occur in nano-particles if the relative interfacial energies change to decrease the dihedral angle during sintering. The model and results will be presented and compared to the experimental results. Furthermore, the implication of these results for sintering will be discussed. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's Nuclear Security Administration under contract DE-AC04-94AL85000.

P3.39

Theoretical Investigation of Elastic/Plastic Deformation During Growth of Strained Si on Si(1-x)Ge(x).

Faouzia Sahtout Karoui, Abdennaceur Karoui and George A. Rozgonyi; Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina.

Strained Si epitaxial layer on SiGe/Si are suitable for high carrier mobility in bipolar transistors. However, film-induced local stresses degrade the structural integrity and the electronic properties of the strained Si film. Quantify and understand the interplay of stresses, defect formation and morphology in SiGe based heterostructures, are essential to lessen the defect distribution at the interfaces and the subsequent defect propagation and interactions. The elastic and plastic stress distribution in strained Si/Si_{1-x}Ge_x (const. x)/Si_{1-x}Ge_x (graded to x) on silicon has been investigated during growth using transient, non-linear finite element modeling. The material plastic behavior is described by the von Mises yield criteria coupled with isotropic work hardening conditions [1,2]. The calculated stress distribution at 1050°C (500 sec.), for x = 0.2 and x = 0.5, shows that the von Mises stress fluctuates strongly within the layers and at the interfaces. The surface of the constant composition Si_{1-x}Ge_x layer is under compressive stress in both cases. Within that layer the normal stress in the growth direction remains compressive for x = 0.2, while it changes from compressive to tensile for x = 0.5. In the graded layer the stress goes from tensile to compressive for x = 0.5 and in the opposite way for x = 0.2. High plastic deformation is observed in the layers being higher for x = 0.5. The maximum plastic stress is localized in the SiGe graded region. The strain profile in the graded layer appeared in good agreement with the anisotropic etching rate profile of this structure [3]. The plastic strain vanishes monotonically up to 8 μm into the Si bulk, in agreement with TEM images that revealed dislocation loops penetrating into the substrate [4]. The time dependent analysis shows that elastic and plastic deformation appear almost instantaneously in the sublayers, while the strain in the Si substrate is delayed up to 300 sec. References [1]: Ansys theory reference manual (Ansys inc.). [2]: W. Schroter, et al, J. Appl. Phys. 54(4), 1816 (1983). [3]: K. Bray et al., Interfaces in Electronic Materials Symp., ECS meeting, Orlando, FL, Oct. 2003. [4]: E A Steinman et al, Semicond. Sci. Technol. 14, 582-588 (1999).

P3.40

Influence of Sol-Gel Chemistry on the Structural Evolution and Mechanical Properties of Nanohybrid Films. Gerard Calleja, Catherine Tartivel, Bruno A. Latella, David J. Cassidy, Christophe J. Barbe and **John Bartlett**; Materials and Engineering Science, Australian Nuclear Science and Technology Organisation, Menai, New South Wales, Australia.

Organic-inorganic nanohybrids obtained by sol-gel processing offer a versatile new approach for fabricating thin films for a wide range of applications, including sensors, waveguides, integrated optics, and corrosion and scratch resistant coatings. A critical issue for technological applications of these coatings is their mechanical behaviour and adhesion to the substrate. By controlling the chemistry of the organic moieties incorporated into the nanohybrids, the mechanical properties of the resulting coatings can be readily modulated. The influence of the connectivity of the inorganic network and the chemistry of the organic modifier on the final mechanical properties of nanostructured coatings on silicon wafers was investigated by spin-coating mixtures of TEOS and 3-glycidoxypropyltrimethoxysilane (GTMS). Processing conditions were chosen to enable the structural evolution of the inorganic and organic networks to be controlled independently. The connectivity of the inorganic and organic networks during processing was investigated by ¹³C- and ²⁹Si-NMR, SAXS, FT-IR and Raman spectroscopy, while the corresponding mechanical properties of the coatings (Young's modulus, hardness and adhesion) were probed via nano-indentation and in-situ tensile testing. The influence of organic chain length and chemical functionality on the structural evolution and mechanical properties of the nanohybrid films was investigated by substituting GTMS with precursors such as methyltrimethoxysilane (MTMS), vinyltrimethoxysilane (VTMS), phenyltrimethoxysilane (PhTMS), n-octyl-tri-ethoxysilane (OTES), and

N-[3-(trimethoxysilyl)propyl]ethylenediamine (TMSPED) and its benzoic acid adduct (which is capable of undergoing self-assembly). The mechanical properties of the coatings were found to be strongly modulated by the size of the organic modifier, with increasing size leading to a corresponding decrease in the Young's modulus. In contrast, only small differences were observed between the mechanical response of films obtained from precursors with similar chain lengths but different chemical functionality. This effect is attributed to nanosegregation of the organic and inorganic domains during the structural evolution of the coatings, which leads to a significant decrease in the long-range connectivity of the network. Increasing the size of the organic substituent promotes nanosegregation. Similarly, increased ageing of nanohybrid coatings obtained from GTMS (leading to more extensive polycondensation) led to a decrease in both the Young's modulus and hardness and to a corresponding increase in the surface roughness. The relationship between the connectivity of the inorganic network, the volume fraction and size of the organic modifier, and the mechanical response will be discussed.

P3.41

Mechanical Properties of Porous Biphasic Tricalcium Phosphate/Hydroxyapatite Nanocomposite Scaffolds for Bone Tissue Engineering. Hassna Rehman Ramay and Miqin Zhang; Materials Science, University of Washington, Seattle, Washington.

ABSTRACT Fabrication of biodegradable scaffolds for load-bearing bone tissue engineering remains a challenge. In this study, we report a novel nanocomposite scaffold consisting of β-tricalcium phosphate matrix and hydroxyapatite (HA) nanofibers. HA nanofibers are prepared using a biomimetic precipitation method. The role of HA nanofibers in enhancing the mechanical properties of the scaffold will be studied. Mechanical compression tests will be performed to evaluate the yield strength, elastic modulus and toughness. The crystal structure and morphology of HA nanofibers will be determined using x-ray diffraction (XRD) and transmission electron microscopy (TEM). Scanning electron microscope (SEM) will be used to examine the morphology and fracture property of the porous scaffolds to reveal the dominant toughening mechanisms. The concept and approach introduced in this study to prepare the biphasic nanocomposite can be applied to other materials for enhancement of porous structures.

P3.42

Nanophases and their stability produced by nanoindentation of crystalline and amorphous Silicon. James S Williams¹, Jodie E Bradby¹ and Michael V Swain²; ¹Department of Electronic Materials Engineering, The Australian National University, Canberra, Australian Capital Territory, Australia; ²Department of Oral Sciences, University of Otago, Dunedin, New Zealand.

Indentation loading of diamond-cubic (Si-I) can cause an intriguing sequence of phase changes under the indenter, including the formation of a metallic phase Si-II, when the hydrostatic pressure exceeds 11 GPa, and a series of crystalline (Si-III and Si-XII) and amorphous phases during unloading. We have shown that, amorphous silicon is also subject to the same series of phase transformations under indentation loading as is Si-I and, furthermore, the process is quite reproducible. Our results show that it is possible to phase transform nanosized volumes of silicon by using an atomic force microscope (AFM) with diamond tips. This paper focuses on the structure and properties of the silicon nanophases produced with an AFM. In particular we examine the conditions under which either crystalline (Si-III/Si-XII) or amorphous silicon is formed as the end phase and explore the stability of such phases during re-indentation and also annealing. We have attempted to model the process to explore nucleation and growth of end phases during unloading.

SESSION P4/N4: Joint Session: Grain Boundaries and Interfaces in Nanoscale Materials
Chairs: Peter Anderson and Valerie Randle
Wednesday Morning, April 14, 2004
Room 3002 (Moscone West)

8:15 AM P4.1/N4.1

Interaction of Extrinsic Dislocations with a Geometrically Necessary Dislocation Boundary using Dislocation Dynamics Simulations. Shafique Khan¹, Hussein M Zbib¹ and Darcy A Hughes²; ¹School of Mechanical and Materials Engineering, Washington State University, Pullman, Washington; ²Center for Materials and Engineering Sciences, Sandia National Laboratories, Livermore, California.

Different types of dislocation structures are produced during deformation of metals, which are important in terms of their effect on the mechanical properties. One of these deformation dislocations structures are nearly planar geometrically necessary boundaries

(GNBs), which accommodate the mismatch in lattice rotation caused by regions of different slip on either side. The internal dislocation structure of a planar dislocation boundary is characterized by the boundary misorientation axis and the boundary normal. In the present studies, the misorientation axis and boundary normal, as determined from experiments, are used to obtain the internal dislocation structure of the GNB. This information is then used to construct a GNB for 3D dislocation dynamics (DD) simulations. Then an extrinsic dislocation moving in the simulation cell under applied stress is allowed to have an interaction with the GNB. These interactions of an extrinsic dislocation with the GNB may include accommodation of the extrinsic dislocation in the GNB and ejection of an intrinsic dislocation from the GNB. Comprehensive results of these interactions will be presented for extrinsic dislocations of different Burgers vectors and character.

8:30 AM *P4.2/N4.2

Deformation mechanism in nanocrystalline fcc metals: bridging experiments with simulations.

Helena Van Swygenhoven, Peter Michael Derlet, Zeljka Budrovic, Abdellatif Hasnaoui and Anders Froseth; Paul Scherrer Institute, PSI-Villigen, Switzerland.

Atomistic simulations have provided unprecedented insight into the structural and mechanical properties of nanocrystalline materials, highlighting the role of the non-equilibrium grain boundary structure in both inter- and intra-deformation processes. One of the most important results is the capability of the nanosized grain boundary to act as source and sink for dislocations. However the extrapolation of this knowledge to the experimental regime requires a clear understanding of the temporal and spatial scales of the modelling technique and a detailed structural characterisation of the simulated samples. In this contribution the dislocation activity suggested by molecular dynamics for three different fcc metals, Al, Cu, Ni and Au are discussed in terms of the inherent restrictions of the technique, in terms of material properties such as the generalized stacking fault energy, in terms of grain boundary structures and last but not least in terms of experimental observations including efforts to bridge simulations to experiments by means of diffraction pattern calculations.

9:00 AM P4.3/N4.3

Structure of dissociated grain boundaries in nanocrystalline gold. Douglas L. Medlin¹, D. Cohen¹, G. Lucadamo¹ and S. M.

Foiles²; ¹Materials Physics Department, Sandia National Laboratories, Livermore, California; ²Materials and Process Modeling Department, Sandia National Laboratories, Albuquerque, NM, New Mexico.

Grain boundaries in low stacking-fault-energy metals can spread, or dissociate, into a three dimensional configuration by the emission of partial dislocations. This phenomenon is of particular importance in nanocrystalline materials because it increases the volume fraction of material associated with interfacial sites and because the constraints of geometric compatibility in such small-grained systems can locally promote the dissociation. Here, through HRTEM observations and atomistic simulations, we consider the structure of dissociated boundaries in nanocrystalline, [110]-textured Au films. In particular, we address the question of how the ordering of stacking fault arrays at dissociated boundaries is related to the crystallographic orientations of the abutting grains. We focus on experimental observation of two important limiting cases: (1) the formation of 9R stacking, corresponding to a stacking every three close-packed planes, and (2) the formation of HCP stacking, which, possessing a "fault" every other close packed plane, possesses the highest possible density of stacking faults. From an analysis of the topological defects required to connect these intergranular layers to the neighboring FCC crystals, we show how these observations, as well as the dissociated boundary structures found at other misorientations, can be understood and predicted from relatively simple geometric considerations. Finally, we analyze how the constraints that arise at boundary junctions affects the separation of the interfacial dislocations. This work is supported by the U.S. Department of Energy under contract No. DE-AC04-94AL85000 by the Office of Basic Energy Science, Division of Materials Science.

9:15 AM P4.4/N4.4

Interactions between Lattice Dislocations and sigma3 Boundaries in Gold. Emmanuelle A Marquis and Douglas L Medlin; Thin Film and Interface Science, Sandia National Laboratories, Livermore, California.

Grain boundary engineered materials are typically processes to contain high densities of first and higher order twin boundaries, which play important roles in improving the material behavior. It is therefore important to understand their behavior during material deformation, and in particular their interactions with gliding lattice

dislocations. In this study, we focus on the interactions between 1/2 <110> lattice dislocations and the 1/6<112> Shockley partial dislocations at sigma 3 boundaries. The resulting defects are dislocations with a Burgers vector equal to 1/3 <111> observed along sigma 3 {111} boundaries and at junctions between sigma 3 {111} and sigma 3 {112} boundaries. Using high-resolution transmission electron microscopy, we characterized these defects in gold thin films with a <101> texture and containing high densities of sigma 3 {111} and {112} twin boundaries. The frequency of observations of these defects suggests their crucial role in the formation and deformation of twin structures. We present a series of micrographs illustrating possible locking mechanisms of twin boundaries involving lattice dislocations. In particular, one mechanism, by which parallel {112} boundaries interact, involves the interplay between the rigid-body translation state across the {112} boundaries and lattice dislocations. This work is supported by the U.S. Department of Energy, in part by the Office of Basic Energy Sciences, Division of Material Sciences, under contract DE-AC04-94AL85000.

9:30 AM *P4.5/N4.5

Slip Transfer across Hetero-Interfaces in two-phase Titanium Aluminum Intermetallics. Jorg M.K. Wiezorek¹, Xiao-Dong

Zhang² and Hamish L. Fraser³; ¹Materials Science & Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania; ²Center for Materials Science, Bose Corporation, Framingham, Massachusetts; ³Department of Materials Science & Engineering, The Ohio State University, Columbus, Ohio.

Two-phase TiAl based intermetallics with microstructures comprising large volume fractions of lamellar grains are promising candidate materials for applications in advanced gas-turbine-engines. The anisotropic mechanical properties associated with the lamellar microstructure are very well documented in the literature. So-called "soft" and "hard" deformation modes can be distinguished. The interfaces between neighboring lamellae of the two constituent phases, tetragonal ordered gamma-TiAl and hexagonal ordered alpha-2 Ti3Al, have been proposed as efficient obstacles for dislocation motion during "hard" mode deformation. Supposedly, the interactions of slip accommodating defects with these hetero-interfaces play an important role in strengthening of lamellar TiAl. The present experimental study used mechanical tests of oriented lamellar grains and detailed transmission electron microscopy to investigate interactions of slip-accommodating defects with these lamellar interfaces. The details of slip transfer across the lamellar hetero-interfaces have been identified, which could provide a basis for modeling the strength of lamellar two-phase TiAl alloys. Thus the role of defect-interactions on the strength and ductility of two-phase TiAl has been elucidated. Support for this work by a grant from the National Science Foundation with Dr. Bruce MacDonald as program manager and from the Office of Research, University of Pittsburgh are gratefully acknowledged.

10:30 AM *P4.6/N4.6

Shear of weak interfaces as a strengthening mechanism in nanoscale layered composites. Richard G Hoagland and John P Hirth; Materials Science and Technology, Los Alamos National Laboratory, Los Alamos, New Mexico.

Resistance to slip through interfaces can take on a variety of forms often involving the internal stresses associated with coherency. But in composites with incoherent interfaces, such as those formed from metals with dissimilar crystal structure or large lattice parameter mismatch, coherent stresses are unlikely although such materials, e.g., Cu/Nb, are still found to achieve very high strength levels. Atomistic simulations of an fcc/bcc system containing incoherent interfaces, reveals that such interfaces shear in response to the stress fields of nearby dislocations. We present these results and show their implications that: 1) a dislocation near an interface is attracted to it, and 2) once in the interface the dislocation core spreads. Both consequences make it difficult for slip to pass through the interface and we suggest that this behavior can explain the origins of strength in systems with incoherent interfaces. We also present a linear elastic model that generalizes the results to enable predictions of the relation of interfacial shear strength to the overall strength of this type of composite. This work was supported by the Office of Basic Energy Sciences, U. S. Dept. of Energy.

11:00 AM P4.7/N4.7

Atomistic Study of Dislocation-Coherent Precipitate

Interaction in Cu-Co Alloys. Jae-Hyeok Shim and Brian D Wirth; Department of Nuclear Engineering, University of California, Berkeley, Berkeley, California.

Introducing precipitates in a metal matrix is an effective means of increasing strength at low and at high temperatures, and of improving high temperature creep behavior. While the general features of

precipitate strengthening that results from coherency strain hardening, chemical hardening and dispersion hardening are well known, many of the detailed interaction mechanisms remain to be determined at the atomic scale. In particular, consider the case of Cu-Co alloys. In these alloys, small ($d < 5$ nm) fcc Co precipitates form which have very strong coherency with the Cu matrix. At larger sizes ($d > 10$ nm), the precipitates transform to the equilibrium hcp structure. Yet, at sizes where the precipitates are believed to all be coherent, anomalous temperature dependence of the yield strength has been observed in Cu-Co alloys [1]. In this work, we use molecular dynamics simulations to investigate the detailed atomistic dislocation-precipitate interactions in Cu-Co alloys. In particular, we report the dislocation bypass mechanism from the precipitates as a function of Co precipitate size, interface coherency and temperature. The simulations have been performed using different parameterizations of the Cu-Co alloy system within the Embedded Atom Method (EAM). The results reveal the effect of the precipitate shear modulus, lattice stability and interface type on the dislocation interactions. 1. N. Buttner and E. Nembach: *Z. Metallkd.*, 76 (1985) 82.

11:15 AM P4.8/N4.8

Dislocation-Twin Interactions in Monazite. Randall Hay, USAF, WPAFB, Ohio.

Monazite (LaPO₄) is monoclinic with lattice parameters $a = 0.683$ nm, $b = 0.706$ nm, $c = 0.648$ nm, and $\beta = 103.2$ degrees. It is refractory (mp 2072°C), relatively soft (5 GPa), machinable, and stable with many common oxides. The mechanical properties of monazite promote distributive damage mechanisms in ceramic composites. Dislocation-twin interactions were identified by TEM in monazite that was spherically indented at room temperature. Emissary lattice dislocations in front of twin tips were observed. Shear of twin lamellae by slip was also observed. Where possible, slip systems were identified. Three types of climb-dissociated partial dislocations were observed. Two types were found on twin boundaries, and a third in the lattice. Formation mechanisms are discussed. Glide of climb dissociated partial dislocations allowed by stacking fault migration is considered. Monazite recovers easily from radiation-induced amorphization at low temperatures. Room-temperature wear of monazite forms fine-grained microstructures that suggest recrystallization. These observations, as well as those presented here for climb-dissociation, suggest that some low-temperature diffusion mechanisms may be faster in monazite than in other refractory oxides.

11:30 AM P4.9/N4.9

The Mechanical Properties in the vicinity of Grain Boundaries in ultrafine-grained and polycrystalline materials studied by Nanoindentations. Elmar Schweitzer and Matthias Goeken; Materials Science, University Erlangen-Nuremberg, Erlangen, Germany.

The strength of structural materials strongly depends on the structure and properties of grain boundaries. Interfaces usually act as barriers to dislocation motion and therefore strengthen materials with decreasing grain size, quantitatively described by the well-known Hall-Petch relation. However, interfaces in nanocrystalline materials are often covered with impurities or second phases, which may influence the mechanical properties. With nanoindentation testing it is now possible to probe the strength of interfaces like grain boundaries directly on a nanometer scale. Therefore this method was used to investigate the properties around grain boundaries in polycrystalline materials with conventional grain sizes and in ultrafine-grained metals prepared by equal channel angular pressing (ECAP), where no impurities are introduced during processing. The results show that strengthening effects of grain boundaries strongly depend on the alloy composition in the vicinity of the boundary. Measurements on an austenitic steel clearly show a decreasing hardness close to the interface in opposite to the general expected behaviour of strengthening. In this case segregation effects strongly influence the mechanical properties around the boundaries. In strongly ordered intermetallics like NiAl no softening or strengthening influence around boundaries was found. The influence of interfaces on the mechanical properties was investigated in materials with grain sizes down to 100 nm and will be discussed in the paper.

11:45 AM P4.10/N4.10

Interfacial properties of a computer generated nanostructured alloy as influenced by the thermodynamics of the classic model used for the interactions. Alfredo Caro, Babak Sadigh and Eduardo Bringa; CMS, LLNL, Livermore, California.

We study the interfacial properties of a computer-generated nano-structured alloy, as influenced by the thermodynamics implicit in the classic model used for the interactions. Metallic alloys are difficult to model with the present level of complexity of empirical potentials because basic thermodynamic properties are absent from

the formulation of these potentials and can only be incorporated in an empirical way, thus introducing uncertainty in the reliability of the predictions. Due to the complexity involved in the calculation of accurate phase diagrams, in most cases the thermodynamics that emerges from these empirical models is unknown. In this work we use our calculated phase diagram of EAM Au-Ni alloys and its interesting property that the excess enthalpy of mixing in the liquid phase is negative, while in the solid solution is positive. We show that the interfacial disordered region of an EAM Au-Ni bulk nano-phase made up of nano grains of pure Au and pure Ni, stabilizes the structure, opening the way to super-plasticity by increasing the energy needed for inter-granular fracture.

SESSION P5: Nanostructured metals and alloys-I
Chairs: Charles Barbour and Helena Van Swygenhoven
Wednesday Afternoon, April 14, 2004
Room 3002 (Moscone West)

1:30 PM *P5.1

Critical Experiments on the Strain Rate Sensitivity and Fatigue Response of Nanostructured Metals and Alloys. Subra Suresh, Timothy Hanlon and Ming Dao; Dept of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Systematic experimental results are presented on the strain rate sensitivity of fully dense, nanocrystalline metals whose mean grain size and range of grain sizes are below 100 nm. The strain rate sensitivity is probed by recourse to two independent experimental methods under different loading conditions. On the basis of these experiments, it is shown that nanocrystalline metals exhibit significantly more pronounced strain rate sensitivity than ultrafine crystalline metals (with a grain size in the range of 100 to 1000 nm) and microcrystalline metals (with a grain size in excess of 1000 nm). Conceptual and quantitative models to rationalize such rate sensitivity are described. Attention is then shifted to the resistance of nanocrystalline metals and alloys subjected to stress-controlled high cycle fatigue as well as to subcritical fatigue fracture. It is shown that while the fatigue life is increased by grain refinement to nanometer size scale, the resistance to fatigue crack growth in nanocrystalline metals and alloys is inferior to that seen in ultrafine crystalline and microcrystalline metals. The effects of different processing conditions on the fatigue response are also systematically explored. Mechanisms responsible for these trends are described.

2:00 PM P5.2

Plastic deformation with a reversible peak broadening in electrodeposited nanocrystalline Ni. Zeljka Budrovic, Helena Van Swygenhoven, Peter Michael Derlet, Steven Van Petegem and Bernd Schmitt; Paul Scherrer Institute, PSI-Villigen, Switzerland.

Electrodeposited nc-Ni and coarse grained Ni are deformed under tensile conditions in-situ in the materials beamline of the Swiss Light Source. As expected for coarse grained materials, peak profile analysis demonstrates that plastic deformation is governed by dislocation mediated processes that accumulate a residual dislocation network producing inhomogeneous strains and an irreversible broadening of the Bragg peaks in X-ray diffraction. On the contrary, the peak broadening during plastic deformation of nanocrystalline Ni is reversible upon unloading, demonstrating that the deformation process does not build up a residual dislocation network. Moreover, no increase in stacking fault density is measured. This new in-situ technique, based on well known peak profile analysis methods, is an important new approach for addressing the relationship between microstructure and mechanical properties in nanostructured materials. The results are discussed in terms of the microstructure and deformation parameters such as strain rate.

2:15 PM P5.3

High strain rate deformation of nanocrystalline metals. Eduardo M Bringa¹, Grant Bazan¹, Alfredo Caro¹, Robert Cavallo¹, Alan Jankowski¹, Stephen Glade¹, James McNaney¹, Bruce Remington¹, Raymond Smith¹, Ben Torralva¹ and Maximo Victoria²; ¹Lawrence Livermore National Laboratory, Livermore, California; ²EPFL, CRPP-Fusion Technology Materials, Villigen, Switzerland.

Recent experimental results in electrodeposited nano-crystalline (nc) Ni (30 nm grain size) deformed up to strain rates of $10^3/s$ [1] show an increase of more than one order of magnitude in both yield strength (Y_s) and strain rate sensitivity. The rate of increase of the Y_s is higher than that of coarse grain Ni for the same strain rates. New developments in laser-driven high strain rate, high pressure materials testing have created a test platform capable of producing controlled pressure pulse with strain rates from $5 \times 10^6/s$ (shockless) up to shock loading conditions. One advantage of using a shockless drive is the

reduction in peak temperature the sample experiences as compared to shock loading. Materials loaded using this drive are routinely recovered for analysis using a number of standard characterizations techniques. I will describe the current Lawrence Livermore National Laboratory effort to study high strain rate deformation of nc Ni, both experimentally, using laser induced shocks and isentropic compression, and theoretically using molecular dynamics simulations and continuum simulations. This will provide novel data since deformation mechanisms under these conditions (strain rates $> 10^6/s$ and grain size < 100 nm) have not been explored before. This effort would provide results for a unique and first time comparison with simulations spanning the relevant length and time scale covered in the experiments. We have already obtained preliminary atomistic simulation results for a nc Cu sample (5 nm grains) under shock loading. Our simulations indicate that deformation occurs at the GB's, and that shock melting occurs at much lower pressures than that for samples with micron size grains. First experimental results are expected in early 2004. [1] F. Dalla Torre, H. Van Swygenhoven, M. Victoria, *Acta Mater* 50, 3957 (2002). 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

2:30 PM P5.4

Experimental Observations of Deformation Mechanisms in Nanocrystalline Metals. Xiaozhou Liao¹, Fei Zhou², Enrique J Lavernia², Yonghao Zhao¹, Srivilliputhur G Srinivasan¹, Michael I Baskes¹, Ruslan Z Valiev³, Dmitry V Gunderov³ and Yuntian Zhu¹; ¹Division of Materials Science and Technology, Los Alamos National Laboratory, Los Alamos, New Mexico; ²Department of Chemical Engineering & Materials Science, University of California at Davis, Davis, California; ³Institute of Physics of Advanced Materials, Ufa State Aviation Technical University, K. Marksa 12, Ufa, Russian Federation.

The microstructures and deformation mechanisms of nanocrystalline Al processed by cryogenic ball-milling and nanocrystalline Cu processed by high-pressure torsion at a very low strain rate and at room temperature were investigated using high-resolution transmission electron microscopy. For nanocrystalline Al, we observed partial dislocation emission from grain boundaries, which consequently resulted in deformation stacking faults and twinning. These results are surprising because (1) partial dislocation emission from grain boundaries has not been experimentally observed although it has been predicted by simulations and (2) deformation stacking faults and twinning have not been reported in Al due to its high SF energy. For nanocrystalline Cu, we found that twinning becomes a major deformation mechanism, which contrasts with the literature reports that deformation twinning in coarse-grained copper occurs only under high strain rate and/or low temperature conditions and that reducing grain sizes suppresses deformation twinning. The investigation of the twinning morphology suggests that the twins and stacking faults in nanocrystalline copper were formed through partial dislocation emissions from grain boundaries. This mechanism differs from the pole mechanism operating in coarse-grained copper.

2:45 PM P5.5

Formation Mechanisms of Deformation Twinning in Ultrafine-Grained Metals. Yuntian Zhu¹, Xiaozhou Liao¹, Srivilliputhur G Srinivasan¹, Yonghao Zhao¹, Michael I Baskes¹ and Enrique J Lavernia²; ¹Division of Materials Science and Technology, Los Alamos National Laboratory, Los Alamos, New Mexico; ²Department of Chemical Engineering & Materials Science, University of California at Davis, Davis, California.

Deformation twins have been experimentally found in nanocrystalline Al and Cu. These twins were found to form via mechanisms that are different from the well-known pole mechanism in coarse-grained fcc metals. This work explores the formation mechanisms of these twins as well as their formation conditions. It presents new critical pieces to the puzzle of deformation mechanisms in ultrafine-grained materials and provides insights into the mechanical properties of ultrafine-grained materials.

3:30 PM *P5.6

Searching for evidence of new deformation mechanisms in nanocrystalline metals. Evan Ma, Materials Sci & Eng, Johns Hopkins University, Baltimore, Maryland.

Computer simulations have predicted that new or unusual deformation mechanisms can emerge when the grain size of nanocrystalline metals is below approximately 30 nanometers. Recently we have carried out experiments, employing extensive transmission electron microscopy as well as temperature and strain rate change tests, to search for evidence of new intra-grain and inter-grain deformation processes that may be operating and rate-controlling. We used truly nanocrystalline, deposited samples of

Al, Ni, Co and Cu. The materials are examined in tensile tests to monitor the yielding and strain hardening behavior. Examples will be presented in this talk to discuss the possible roles of partial dislocations, twinning, Coble creep, and grain boundary sliding.

4:00 PM P5.7

Relating the Dimensionality of Internal Nanostructures to the Mechanical Properties of Metals. David M. Follstaedt, James A. Knapp and J. Charles Barbour; Physical and Chemical Sciences Center, Sandia National Laboratories, Albuquerque, New Mexico.

Several mechanisms are known to strengthen metals with refined internal structures, such as dislocation pinning by precipitates and inhibited slip transfers across grain boundaries, twin planes, and interfaces. Small grains produce high strength in deposited layers, but fine-scale twinning is also proposed to be important for determining strength. We have used nanoindentation to examine the hardness of Ni layers produced by pulsed laser deposition and found a Hall-Petch relationship over a wide range of lateral grain sizes, from 600 nm down to 10 nm. The smallest grains are in thin layers (50-70 nm) deposited at room temperature and appear equiaxed. Thick layers (500 nm) deposited at room temperature with lateral sizes 30 nm show some degree of columnar growth, while layers deposited at 275°C have wider (120-160 nm) columnar grains that extended across the layer. In spite of this 1D columnar nature, the Hall-Petch relationship is obtained using only lateral grain width as the critical dimension, with the resulting slope ($H = kd^{1/2}$) agreeing with that for micrometer-size Ni grains. This result can be understood for randomly oriented grains and dislocation glide planes, since the average length of a randomly oriented chord through a columnar grain changes slowly with aspect ratio. We are currently examining Cu layers with lateral grain sizes 110 nm. Layers deposited at room temperature show (111) texture and extensive twinning on planes nearly parallel to the substrate and surface, with spacings 4-40 nm. Such twinning is absent in Cu layers deposited at 200°C, allowing us to compare the effect of this 2D nanostructuring on hardness. Preliminary results suggest limited changes in hardness with twinning. We are using finite-element modeling to explore the orientation of indentation shear stresses relative to the internal structures, which may relate dimensionality and orientation of nanostructures to measured mechanical properties. This work was supported by the DOE Office of Basic Energy Sciences. Sandia is a multiprogram laboratory operated by Sandia Corporation under contract DE-AC04-94AL85000.

4:15 PM P5.8

Elevated Temperature Mechanical Properties of Devitrified Metallic Glass. Nathan Allan Mara, Alla V Sergueeva and Amiya K Mukherjee; Chemical Engineering and Materials Science, University of California, Davis, Davis, California.

Elevated temperature tensile tests of different microstructures arising from different heat treatments of the Fe-based metallic glass Vitroperm ($Fe_{73.5}Cu_1Nb_3Si_{15.5}B_7$) are presented. An anneal at 600°C for 1h yields a single phase α -Fe microstructure with equiaxed, randomly oriented 15 nm grains, which is an ideal candidate for study of material properties at diminishing length scale. This microstructure has good stability during tensile testing at 600°C, showing a strain rate exponent correlating to grain boundary sliding ($m=0.5$), but little ductility, and strengths to 1250 MPa. The brittle behavior could be attributed to the lack of dislocation activity at such length scales. At temperatures up to 725°C, grain growth occurs, leading to elongations as large as 65% at flow stresses of 250 MPa. Precipitation of a second Nb-rich phase accompanies the grain growth. This investigation is supported by NSF, Division of Materials Research, grant NSF-DMR-0240144.

4:30 PM P5.9

The Relationship Between Crystallite Size, Texture, Mechanical Strength, and Mn Content in Dilute Electrodeposited NiMn Alloys. Alec Talin, Steven Goods, James Kelly, Scott Spangler, Emmanuelle Marquis and Gene Lucadamo; Sandia National Labs, Livermore, California.

Ultrafine grain Ni produced by electrodeposition is a promising structural material for a variety of applications requiring high mechanical strength and hardness. Potential applications include CD stampers, MEMS, and high aspect ratio microsystem components/LIGA. The principal drawbacks of ultrafine grain Ni are its low recrystallization temperature ($\approx 200^\circ\text{C}$) resulting in loss of strength and its propensity to suffer sulfur-induced intergranular fracture after exposures to quite modest temperatures (also about 200°C). Electroplated NiMn alloys exhibit average grain size below 30 nm, yield strength in excess of 1 GPa and are stable with respect to one hour thermal anneals at 400°C. The Mn^{++} ion acts as a grain refiner in a fashion similar to that of organic additives, such as saccharin, commonly used in Ni-Watts baths. The superior retention of mechanical strength is largely due to the suppression of

recrystallization of Ni by Mn. In this paper we report on the variation of crystallite diameter, crystallographic texture, and yield strength of NiMn electrodeposits as a function of Mn content from 0 wt. % to 1 wt. %. Over this concentration range, Mn reduces the average crystallite size from hundreds of nanometer to 20 nm, changes the texture from a sharp <100> to a <110> orientation, and increases the yield strength from 300 MPa to over 1 GPa. We also show how small additions of Mn solute affects the recrystallization temperature and texture of Ni, and how these results can be understood in terms of the spatial distribution of Mn in Ni, obtained using three dimensional atom probe technique.

4:45 PM P5.10

Microstructural Evolution During Recovery and Recrystallization of Nanocrystalline Al and Al-Mg Alloy Prepared by Cryogenic Ball Milling. Fei Zhou¹, Xiaozhou Liao², Yuntian Zhu², Enrique J. Lavernia³ and Steve R. Nutt¹; ¹Materials Science, University of Southern California, Los Angeles, California; ²Division of Materials Science and Technology, Los Alamos National Laboratory, Los Alamos, New Mexico; ³Chemical Engineering and Materials Science, University of California, Davis, California.

Nanocrystalline Al and Al-7.6 at% Mg alloy powders, consisting of both equiaxed and elongated grains with an average size of 25 nm, were prepared by ball milling at cryogenic temperature. Novel defects, such as high-density dislocations and twins, were revealed in the as-milled samples. The microstructural evolution during thermal annealing of the as-milled samples was examined in detail using differential scanning calorimetry, x-ray diffraction and transmission electron microscopy. Recovery occurs at temperatures from 100 to 230 °C, resulting in significant strain relaxation and grain coarsening in the samples. Recrystallization proceeds at higher temperatures with further grain growth. The stored enthalpy release during recovery was found to be significantly larger than that in coarse-grained Al and Al alloys deformed by other cold-working methods. The origin of the measured enthalpy was analyzed. Both recovery and recrystallization give rise to non-uniform microstructures with bimodal grain size distributions, which are in the range from nanoscale (30 to 50 nm) for ultrafine grains to sub-microscale (300 to 500 nm) for coarse grains. The microscopic observations indicate that grain coalescence is a feasible mechanism for coarsening associated with the recovery.

SESSION P6: Mechanical Behavior at the Nanoscale:
Theory, Modeling and Simulation
Chairs: Vasily Bulatov and Robert Rudd
Thursday Morning, April 15, 2004
Room 3002 (Moscone West)

8:15 AM P6.1

Mechanism-based strain gradient crystal plasticity. Chung-Souk Han^{2,1}, Huajian Gao¹, Yonggang Huang³ and William D. Nix²; ¹Max Planck Institute for Metal Research, Stuttgart, Germany; ²Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305, California; ³Department of Mechanical and Industrial Engineering, University of Illinois, Urbana, IL 61801, Illinois.

We have been developing the theory of mechanism-based strain gradient plasticity (MSG) to model size dependent plastic deformation at micron and submicron length scales. The core idea has been to incorporate the concept of geometrically necessary dislocations into the continuum plastic constitutive laws via the Taylor hardening relation. Here we extend this effort to develop a mechanism-based strain gradient theory for crystal plasticity (MSG-CP) based on the notions of dislocation density tensor and resolved density force corresponding to the Peach-Koehler force in dislocation theory. The framework of large deformation continuum crystal plasticity is adopted, and the material formulation is considered in the intermediate configuration under the assumption of small elastic strains. An effective density of geometrically necessary dislocations is defined on the basis of resolved density force for specific slip systems and is incorporated into the plastic constitutive laws via the Taylor relation.

8:30 AM *P6.2

Rupture of a Thin Metal Film on a Polymer Substrate. Zhigang Suo, Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts.

Under tension, a freestanding thin metal film usually ruptures at a much smaller strain than its bulk counterpart. Often this apparent brittleness does not result from cleavage, but from strain localization, such as local thinning. By volume conservation, local thinning causes local elongation, which is accommodated as the ruptured halves move apart. Now consider a weakly hardening metal film on a steeply

hardening polymer substrate. If the metal film is fully bonded to the polymer substrate, the substrate suppresses large local elongation in the film, so that the metal film may deform uniformly to large strains. If the metal film debonds from the substrate, however, the film becomes freestanding and ruptures at a smaller strain than the fully bonded film. We study strain delocalization in the metal film on the polymer substrate by analyzing incipient and large-amplitude nonuniform deformation, as well as debond-assisted necking. The theoretical considerations call for further experiments to clarify the rupture behavior of the metal-on-polymer laminates. This work is carried out in collaboration with T. Li, Z.Y. Huang, Z.C. Xi, S. P. Lacour, S. Wagner. A preprint is available at <http://www.deas.harvard.edu/suo/>, Publication 148.

9:00 AM P6.3

Hyperelastic effects in brittle materials failure. Markus J Buehler¹, Farid F Abraham² and Huajian Gao¹; ¹Gao, Max Planck Institute for Metals Research, Stuttgart, Germany; ²IBM Almaden Research Laboratory, San Jose, California.

The elasticity of a solid clearly depends on its state of deformation. Metals will weaken, or soften, and polymers may stiffen as the strain approaches the state of materials failure. It is only for infinitesimal deformation that the elastic moduli can be considered constant and the elasticity of the solid linear. However, many existing theories model fracture using linear elasticity. Certainly, this can be considered questionable since material is failing at the tip of a dynamic crack because of the extreme deformation. We show by large-scale atomistic simulations that hyperelasticity, the elasticity of large strains, can play a governing role in the dynamics of fracture and that linear theory is incapable of capturing all phenomena. We propose a simple biharmonic interatomic potential suitable for a systematic study of hyperelastic effects in dynamic fracture. The main result of this paper is the new concept of a characteristic length scale χ for the energy flux near the crack tip. We demonstrate that the local hyperelastic wave speed governs the crack speed when the hyperelastic zone approaches this energy length scale χ . This allows for super-Rayleigh and intersonic mode I cracks, as well as supersonic mode II cracks. The length scale χ is proportional to the fracture surface energy and Young's modulus, and inverse proportional to the square of the applied stress. We show that the length scale χ , heretofore missing in the existing theories of dynamic fracture is helpful in forming a comprehensive picture of crack dynamics. An important result is that the effect of hyperelasticity is important for nanoscale materials, such as highly strained thin films or nanostructured materials, as well as high speed impact phenomena. This is because the characteristic length scale χ becomes small due to large applied stresses. However, in most engineering and geological applications the effect of hyperelasticity is negligible since the applied stress is low and χ gets large. It is well known that dynamic cracks feature a dynamic instability. For low velocities, the crack surface is perfectly smooth but gets rough at high propagation speeds. The speed at which this transition occurs is referred to as the critical crack speed for the instability. We investigate the effect of hyperelasticity for this critical crack speed. First we show agreement of cracks in harmonic lattices with the Yoffe criterion, a linear continuum mechanics theory. We illustrate that a softening hyperelastic effect leads to a decrease in the critical crack speed for the instability, and a stiffening hyperelastic effect leads to an increase in the critical speed, in contradiction to the classical linear continuum mechanics theories. The observations in MD simulation are critically discussed with respect to relevant experimental results. The main conclusion is that hyperelasticity plays a critical role in understanding experimental and computational observations in brittle fracture.

9:15 AM P6.4

Short Chains of Copper Nanoparticles under Mechanical Strain - A Molecular Dynamics Study. Adamos Dalis and Sheldon Friedlander; Chemical Engineering Dept, UCLA, Los Angeles, California.

Previous studies in our laboratory have shown that individual nanoparticle chain aggregates (NCA) exhibit interesting mechanical behavior when under strain inside the transmission electron microscope. NCA made of various materials (e.g. carbon, metal oxides, metals, etc.) were strained by as much as 100% when tension was applied to them. After breaking, the NCA rapidly contracted to form more compact structures. In this study, molecular dynamics (MD) computer simulations are employed to investigate, at the atomic scale, the behavior of short nanoparticle chains under strain and to obtain quantitative information of the forces involved in chain straining and fracturing. The interaction potential used is that of copper obtained with the embedded atom method (EAM). Copper is selected as a test material because reliable interatomic potentials are available. Six to eight single-crystal nanoparticles, each of about 2.5 nm in diameter, are placed in contact in various chain configurations. The structures are initially relaxed adiabatically with MD steps for

200 ps, at a starting temperature of 300 K. The bonding energy between any two nanoparticles in contact is about 30 eV at 0 K. The relaxed chain configurations are strained along their longest dimension, to the breaking point, at strain rates spanning from 0.3 m/s to 10 m/s. We identify mechanisms of stress accommodation that lead to plastic deformation and eventually fracture. After an initial almost purely elastic straining of about 8% kinked portions of the chains start to straighten. This is done by a combination of particle-particle rotation and interface sliding, during which the stress along the straining axis remains largely unchanged at about 1.5 GPa. The initial chain straightening compares well with the experimental observations. Once the nanoparticle rotation is completed, the stress increases further to reach a maximum of about 4 GPa. At about 40% strain, repeated slip events on {111} planes cause the neck region between two nanoparticles to decrease in size to the point where it reduces to a single atom contact. Eventually, the single atom contact yields and the chains break at a strain of about 50%. Applications of our experimental and simulation studies on NCA are to nanocomposite materials, including carbon black reinforced rubber.

9:30 AM P6.5

Nanoscale Structure and High Velocity Sliding at Cu/Ag Interfaces. James E. Hammerberg,¹ Applied Physics Division, Los Alamos National Laboratory, Los Alamos, New Mexico; ²University of Texas, El Paso, El Paso, Texas; ³Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico.

We present the results of large-scale Non-Equilibrium Molecular Dynamics (NEMD) simulations for Cu/Ag interfaces sliding in the velocity regime $0 < v \leq 1$ km/s. System sizes up to 5.5 million atoms are considered using Embedded Atom Method (EAM) potentials. Sliding of single crystals with (100) and (111) faces are considered. We discuss the observed velocity weakening in the tangential force and its connection with the observed dislocation structures and nanostructure that are nucleated during dry sliding.

9:45 AM P6.6

Nanoindentation and incipient plasticity: effects of temperature. Laurent Michel Dupuy¹, Ron Miller² and Rob Phillips¹, ¹Mechanical Engineering, California Institute of Technology, Pasadena, California; ²Department of Mechanical and Aerospace Engineering, Carleton University, Ottawa, Ontario, Canada.

Nucleation and kinetics of defects at the atomic scale provide fundamental information about the mechanical behavior of crystalline materials. Nanoindentation experiments and simulations have demonstrated in the past the potential to probe these mechanisms. The effects of temperature are addressed numerically in this presentation. The Quasicontinuum method was recently extended to study the dynamical properties of defects in materials at finite temperature. It allows to simulate large systems with an atomistic resolution without the overwhelming computational cost associated to full molecular dynamics simulations. Explicit dynamical simulations are carried out on incipient plasticity during nanoindentation tests in Nickel. We obtain both macroscopic load versus indentation depth curves, as well as information regarding the atomistic mechanisms as a function of temperature: the nucleation of dislocations, their propagation and the Peierls stress. These simulations reveal a strong dependence of the critical stress to nucleate dislocations on the temperature.

10:30 AM P6.7

Atomistic Simulations of Dislocation-Interface Interactions in Thin Films. Y.-L. Shen, Mechanical Engineering, University of New Mexico, Albuquerque, New Mexico.

This study focuses on the atomistics of thin-film plasticity and the interaction of dislocations with interfaces. Special attention is devoted to the effect of atomic sliding capability at the interface between a plastically deforming film and a stiff adjacent layer. Molecular statics simulations were carried out to corroborate the overall film response and the nano-scale defect mechanisms. A free-sliding interface is shown to be able to "reflect" oncoming dislocations and enhance film plasticity. A rigidly bonded interface, on the other hand, is seen to resist approaching dislocations. Partial sliding results in a transitional behavior between the two extremes, as revealed in our parametric analysis. The sliding capability of interface atoms is also seen to dictate the overall film strength.

10:45 AM P6.8

The effects of grown-in twins on the deformation mechanism of nc-Al, Ni and Cu: a molecular dynamics simulation. Anders Froseth, Peter Michael Derlet and Helena Van Swygenhoven; Paul Scherrer Institute, PSI-Villigen, Switzerland.

Studies of deformation mechanics by means of molecular dynamics computer simulations have been until now only performed on

nc-samples with defect free grains. Simulations of fully 3D-GB networks have shown that from a certain grain size on, the nc-GBs act as source and sink for dislocations. TEM analyses of experimental samples however often evidence the presence of grown-in twins in the small grains, their number depending on the synthesis technique and synthesis parameters. In this contribution we investigate the effect of grown in twins on the deformation behaviour of nanocrystalline Al, Ni and Cu using molecular dynamics simulations. It is shown that in the presence of grown-in twins, plastic deformation is enhanced and results, in part, from twin-boundary migration in which partial dislocations emitted at the intersection of the twin boundary and the GB travel through the entire grain. A comparative study of Al, Ni and Cu is performed that shows that the rate of twin migration is determined by the characteristics of the generalized stacking and twinning fault energy curves of the material.

11:00 AM P6.9

Modeling of High Strain Rate Deformation and Strain Localization in FCC Single Crystals: Dislocation Dynamics Analyses. Mutasem A Shehadeh¹, Hussein Zbib¹, Tom de la Rubia² and Vasily Bulatov²; ¹Washington State University, Pullman, Washington; ²Lawrence Livermore National Laboratory, Livermore, California.

This research intends to develop better understanding of the high strain rate deformation in the micro length scale by investigating the interaction between stress waves and dislocations. A multiscale dislocation dynamic plasticity model that couples dislocation dynamics and finite element analyses is used to simulate the loading conditions of the recent laser based experiments in which the pulse duration is in the order of few nanoseconds. In this work, the effects of several stress wave and material parameters on the deformation process in FCC single crystals are analyzed. The effects of strain rate, shock pulse duration, rise time, crystal anisotropy and the pressure dependent elastic properties on the wave profiles and dislocation microstructures are investigated. In addition, the effects of different dislocation dynamics and finite element boundary conditions are studied. The relaxed configurations of dislocation microstructures show the formation of micro bands and dislocation entanglements whose characteristics are strain rate and pulse duration dependent. Moreover, criteria for homogenous nucleation of dislocations and shear banding formation are implemented.

11:15 AM P6.10

Massively Parallel Dislocation Dynamics and Crystal Plasticity. Wei Cai, Vasily V Bulatov, Tim G Pierce, Masato Hiratani, Moono Rhee and Meijie Tang; Chemistry and Materials Science, Lawrence Livermore National Lab, Livermore, California.

Prediction of the plastic strength of single crystals based on the collective dynamics of dislocations has been a grand challenge for computational materials science for a number of years. The difficulty lies in the inability of the available dislocation dynamics (DD) codes to handle a sufficiently large number of dislocation lines, in order to be statistically representative and to reproduce experimentally observed microstructures. Our new massively parallel DD code is capable of modeling million dislocations simultaneously by employing thousands of processors. We will discuss the methods that make simulations of such scale possible. Simulation data on strain hardening and spontaneous dislocation patterning in FCC and BCC metals will be presented and compared with experiments. We will discuss what sort of new information can be extracted from such simulations and examine how close we are able to come to understanding single crystal plasticity from the underlying collective motion of dislocations. 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.

11:30 AM P6.11

Image stresses and dislocation dynamics simulations in nanoscale systems. Meijie Tang, Lawrence Livermore National Lab., Livermore, California.

The existence of free surfaces has a dominating effect to the mechanical properties in nanoscale systems. The image stresses due to the free surfaces are significant and may play a crucial role in the dynamics of dislocations. We developed a dislocation dynamics (DD) simulation code that is coupled with finite element method (FEM) to deal with the image stresses. In particular, a highly efficient and accurate algorithm is developed that utilizes an analytical solution for the singular stress fields around dislocations intersecting the free surfaces. This advanced algorithm allows us to account for the surface image stresses accurately with rather coarse meshes. Some applications on metallic thin film or nano-plate will be discussed. The work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National

11:45 AM P6.12

The Effects of Grain Size on the Strengthening Behavior of Polycrystals: The Dislocation Density Tensor Approach.

Bulent Biner, Materials & Engineering Physics, Ames Laboratory, Ames, Iowa.

In this study, a dislocation pile-up model based on the dislocation density tensor approach was implemented into a 2D finite element code. The analyses were confined to a single slip system and the evolution of the flow stress for grain sizes ranging from about 160 micron to 75 nanometers under shear deformation was examined. The results obtained from these analyses were also compared with the results those obtained from 2D discrete dislocation simulations. Both approaches gave almost identical stress-strain curves and dislocation densities for similar grain sizes. For the grain size ranges considered, an inverse relationship between the grain size and 0.2 percent offset flow stress in the form of Hall-Petch relationship $[d]^{1/2}$ was observed. The evolution of flow stress follows a narrow band when expressed as a function of dislocation density and hence suggests a scaling with the grain size as seen in our earlier studies. The computational aspects of the both approaches will also be discussed. This work was performed for the United States Department of Energy by Iowa State University under contract W-7405-Eng-82. This research was supported by the Director of Energy Research, Office of Basic Sciences.

SESSION P7: Nanocomposites and Nanolaminates
Chairs: Timothy Foecke and Richard Hoagland
Thursday Afternoon, April 15, 2004
Room 3002 (Moscone West)

1:30 PM *P7.1

Processing and Characterization of Nanocrystalline Metallic and Ceramic Materials with Interesting Mechanical Electrical and Thermal Properties. Amiya K. Mukherjee, Chemical Eng & Materials Sci, University of California, Davis, California.

Nanocrystalline materials have been produced by severe plastic deformation, electrodeposition, magnetron sputtering, and crystallization from bulk metallic glass, ball-milling, and powders produced from inert gas condensation. The consolidation of the powder particles in some of these processing routes was achieved by electrical field assisted sintering with capability of superimposing 2 GPa gas pressure. The nanocrystalline metallic materials demonstrated both high strain-rate superplasticity and low-temperature superplasticity with important differences in mechanistic details from their microcrystalline counterparts. The nanomaterials derived from metallic glass showed extreme strength and at elevated temperature superplasticity-like ductility. A three-phase alumina based nanoceramic demonstrated superplasticity at lower temperature and higher strain rate. An alumina-carbon-nanotube-niobium nanocomposite has a fracture toughness that is five times that of pure alumina and an electrical conductivity that is 13 orders of magnitude greater than that for pure nanocrystalline alumina. A silicon nitride/silicon carbide nanocomposite produced by pyrolysis of liquid polymer precursor has produced one of the lowest creep rates in ceramics at a (referred) temperature of 1400°C. These results will be discussed in the context of predictions of recent results from molecular dynamics simulation. This effort is supported by NSF/DMR/Metal, ONR, and ARO with Dr. J. Akkara, Dr. L. Kabacoff, and Dr. W. Mullins as Program Managers, respectively.

2:00 PM P7.2

Molecular Bridging As A Toughening Mechanism For Nanoporous MSSQ. Reinhold Dauskardt¹, Dan Maidenber¹, Robert Miller² and Willi Volksen²; ¹Materials Science, Stanford University, Stanford, California; ²IBM-Almaden Research Center, San Jose, California.

From biological scaffolds to dielectric layers, nano-templated organic-inorganic hybrid glasses are being developed to provide a versatile class of highly porous materials with tunable properties. These glasses are proposed solutions for a variety of thin film devices, from dielectric layers in microelectronics to functional membranes in biological sensor applications. However, the mechanical properties of these low-density brittle glasses is expected to catastrophically deteriorate with the incorporation of nanoporosity. In particular, the adhesion and cracking behavior of the nanoporous glasses is paramount. In this study, we demonstrate remarkable toughening behavior in highly porous Methylsilsesquioxane (MSSQ) films attributed to molecular bridging by molecular remnants of the pore-generating copolymer. Adhesion data at several selected interfaces is presented as a function of porosity for different

porogen-matrix systems. Interfacial toughening was reported for nanocomposites in which the porogen did not totally volatilize. This resulted in increasing adhesion energy at an MSSQ-Silica interface with increasing porosity. X-ray and infrared spectroscopy clearly show remnants of the porogen molecule at the interface. A molecular bridging model is used to explain increases in the adhesion energy of up to 1000%. Implications of this study pertaining to microelectronics and nanocomposite architecture are discussed.

2:15 PM P7.3

Fabrication Process and Mechanical Properties of Carbon Nanotube/Alumina Nanocomposite by Molecular Level Mixing Process. Seung-II Cha, Kyung-Tae Kim, Chan-Bin Mo, Kyong-Ho Lee and Soon-Hyung Hong; Materials Science and Engineering, Korea Advanced Institute of Science and Technology, Daejeon, South Korea.

Carbon nanotubes (CNTs), since their first discovery, have been considered as new promising materials in various fields of applications including reinforcements in composites due to their extra-ordinary properties. In spite of successful development of carbon nanotube reinforced polymer matrix nanocomposites, the researches on carbon nanotube reinforced inorganic matrix nanocomposites such as CNT/ceramic or CNT/metal show limitations due to a difficulty in homogeneous distribution of carbon nanotubes within inorganic matrix. In this study, the carbon nanotube reinforced alumina matrix nanocomposite was fabricated by novel process, molecular level mixing process, and followed by spark plasma sintering process. The molecular level mixing process, which consists of dispersion of CNT within solvent into suspension forms, mixing CNT suspension with Al ions by resolving Al containing chemicals such as $Al(NO_3)_3$ and following oxidation and calcinations, can produce the carbon nanotube/alumina composite powder where the carbon nanotubes are homogeneously implanted in the alumina matrix powder. The CNT/alumina composite powders were consolidated by spark plasma sintering. The CNT/alumina nanocomposites can be consolidated with full densification by spark plasma sintering process at the temperature over 1400°C under a pressure of 40MPa. Both hardness and fracture toughness of carbon nanotube reinforced alumina nanocomposite increases with increasing the volume fraction of carbon nanotubes. At the fracture surface of CNT/alumina nanocomposite, the pulled-out carbon nanotubes, which is generally distributed inside the alumina grains homogeneously, can be observed. This observation shows that the hardness of carbon nanotube reinforced alumina nanocomposite was improved by load transfer from matrix to carbon nanotubes and the fracture toughness was improved by bridging and pull-out of carbon nanotubes.

2:30 PM P7.4

Processing and Mechanical Properties of Nanostructured Yttria-Zirconia Ceramics. Jianyi Cui¹ and Jackie Y Ying^{2,3};

¹Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; ²Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; ³Institute of Bioengineering and Nanotechnology, Singapore Science Park II, Singapore.

Nanostructured ceramics exhibit interesting mechanical phenomena such as improved hardness and bending strength. However, due to the processing challenges of nanostructured ceramics, the mechanism underlying such phenomena remains unclear. In this work, we have investigated the processing of submicron and nanocrystalline 3% yttria-doped zirconia ceramics. The effect of powder characteristics and sintering conditions on the microstructure of sintered bodies was examined. The ceramic grain size was systematically controlled so that mechanical properties can be elucidated as a function of grain size. Nanoindentation as well as bending and wear tests have been performed. Nanostructured ceramics are shown to exhibit superior strength and fracture toughness.

2:45 PM P7.5

Improved Fracture Toughness in Advanced Nanocrystalline Ceramic Composites. Joshua David Kuntz, Guo-Dong Zhan and Amiya K. Mukherjee; Chemical Engineering & Materials Science, University of California - Davis, Davis, California.

Nanocrystalline materials have demonstrated very interesting changes in physical, chemical and mechanical properties at severely diminished length scales. This article focuses on the topic of nanocrystalline ceramic composites specifically designed for applications requiring improved fracture toughness. The difficulty in producing fully consolidated ceramic composites that retain a nanocrystalline structure is the main hurdle for thorough investigations in this area. This obstacle has been overcome in the current investigation through the use of a fast, comparably lower temperature, sintering technique e.g., Spark Plasma Sintering. Alumina based nanocomposites incorporating carbon nanotubes and additionally incorporating

nanocrystalline niobium have yielded fracture toughness values that have exceeded that for pure nanocrystalline alumina by more than 300%. This introduces the question of whether this improvement is merely additive or evidence of a synergistic toughening mechanism involving ductile phase and fiber toughening. This research is supported by grants from the U.S. Army Research Office (G-DAAD19-00-1-0185) with Dr. William Mullins as the Program Manager.

3:30 PM *P7.6

Anelastic and Fatigue Behavior of Metallic Multilayered Thin Films. R.C. Cammarata, Department of Materials Science and Engineering, Johns Hopkins University, Baltimore, Maryland.

It is well known that metallic multilayered thin films have displayed enhancements in such properties as hardness, yield strength, and fracture. In addition to these "static" properties, recent investigations on electrodeposited Cu-Ni multilayered films have shown that they display enhancements in "dynamic" behavior such as internal friction (damping capacity) and fatigue resistance. Results from internal friction testing of free-standing membranes and fatigue studies of bulk copper coated with multilayered films will be presented. The internal friction enhancements appear to be associated with certain relaxation processes, while the fatigue behavior appears to result from suppression of surface crack nucleation.

4:00 PM *P7.7

Effect of Nanolayered Coatings on Fatigue Life in Steel. Julia R. Weertman, MS&E Department, Northwestern University, Evanston, Illinois.

Previous investigators (M Stoudt et al.) have shown the nanolayer coatings of Cu/ Ni on Cu samples can greatly improve fatigue life. In the present case we have carried out fatigue testing on steel samples coating with alternating nanolayers of Cu and Nb and compared the results with fatigue life of uncoating samples. Microstructural changes in the two sets of samples will be described. Research funded by US Department of Energy, Grant DE-FG02-02ER46002/A001

4:30 PM P7.8

Thermomechanical properties and fatigue of nanocrystalline Ni/Cu electrodeposits. Olivier Arnould, Julien Jumel, Olivier Hubert and Francois Hild; LMT Cachan, Cachan, France.

This study deals with the long-term life reliability of a high precision pressure sensor. It uses bellows made of Ni/Cu/Ni layered material (overall thickness 100 μ m) obtained by electrodeposition. Their mechanical stiffness is mainly given by the Ni layers (overall thickness 40 μ m). Ni deposits are obtained in a sulfamate bath. They are made of porous micrometre columnar clusters of low-misoriented (sub)grains (average grain size 60nm) with a low <110> fiber texture aligned along the deposition direction. Thermomechanical properties of these layers are obtained by several techniques (e.g., XRD, tensile test, photothermal microscopy) and compared to theoretical models (e.g., Hall-Petch relationship), computations (e.g., self-consistent elastic homogenization) and other authors' results. Bellows are expected to stay in service for many decades, thus their high cycle fatigue behavior has to be known. A specific fatigue test setup has been designed using a resonant high-cycle fatigue machine. It allows for a simultaneous testing of ten samples at a frequency of 100Hz. Abnormal fatigue crack propagation and stress-life fatigue curve for the crack initiation of the electroplated Ni are measured and identified using numerical computations (i.e., finite element analysis). Stress-life fatigue curves are modeled with a Weibull probabilistic approach associated with a Stromeyer law. Results are compared with other ones obtained on Ni electrodeposits. No specific nanosize effects are observed (when normalized by the yield strength).

4:45 PM P7.9

Ultrasonic-based In-situ Processing of Aluminum Matrix Nano-Composites. Xiaochun Li, Mechanical Engineering, University of Wisconsin-Madison, Madison, Wisconsin.

Lightweight Metal Matrix Nano-Composites (MMNCs) (metal matrix with nano-sized ceramic particles) promise to improve performance of lightweight mechanical systems significantly. It would be desirable to produce high performance as-cast lightweight components of MMNCs. However, it is extremely difficult to disperse nano-sized ceramic particles uniformly in metal melts. High-intensity ultrasonic waves could effectively disperse nanoparticles into alloy melts, making the production of as-cast high performance lightweight MMNCs feasible. The study is to investigate fundamental issues on the ultrasonic non-linear effects during in-situ processing of MMNCs. An ultrasonic-based processing system was developed and used for in-situ processing of MMNCs (Al nano-sized SiC). Physical and mechanical properties of as-cast lightweight MMNCs were evaluated. With a small fraction of nano-sized SiC, as-cast aluminum matrix nanocomposites

demonstrated reproducible microstructures and superior properties. Non-linear ultrasonic effects/microstructure/property relationships are also investigated. The ultrasonic-based method is promising to produce lightweight MMNCs with good reinforcement distribution and sound structural integrity.

SESSION P8: Poster Session: Nanoscale Mechanical Behavior

Thursday Evening, April 15, 2004

8:00 PM

Salons 8-9 (Marriott)

P8.1

A Common Misunderstanding on the Nanoindentation Theory. Guanghui Fu¹ and Anthony C. Fischer-Cripps²; ¹Lam

Research Corporation, Fremont, California; ²Division of the Telecommunications and Industrial Physics, CSIRO, West Lindfield, New South Wales, Australia.

Sneddon's solution on the indentation of an elastic half-space with a rigid conical indenter has been the basis of nanoindentation data analysis for more than a decade. In their finite element simulation, Hay, Bolshakov and Pharr find that Sneddon's solution is not an exact representation of the actual contact. Both the indenter shape and Sneddon's solution have to be modified before it can be used in the interpretation of nanoindentation data (Hay, J.C., Bolshakov, A. and Pharr, G.M., 1999, "A Critical Examination of the fundamental relations used in the analysis of nanoindentation data," Journal of Materials Research, Vol. 14, No. 6, pp. 2296-2305). This contradiction is investigated in this paper. We find Hay et al's conclusion is correct and Sneddon's boundary conditions do not represent the actual contact. Because the half-space surface points in the contact region move ONLY along the indenter surface in a real contact, the r-displacement and z-displacement of those points are coupled. However, Sneddon's boundary conditions only specify the z-displacement. Sneddon's way of giving boundary conditions is common in contact mechanics: people only specify the z-displacement for rigid punch problems and take it for granted that the final surface shape in the contact area is the same as that of the punch. The correct boundary conditions for the actual contact are presented in this paper. These boundary conditions can be changed exactly to Sneddon's boundary conditions if there is no r-displacement. It can also be changed approximately to Sneddon's boundary conditions if the half-included angle of the cone is near 90, i.e., within the limit of the linear elasticity.

P8.2

Analysis of a one-billion atom simulation of work-hardening in ductile materials. Markus J Buehler¹, Alexander Hartmaier¹, Farid F Abraham² and Huajian Gao¹; ¹Gao, Max Planck Institute for Metals Research, Stuttgart, Germany; ²IBM Almaden Research Center, San Jose, California.

The plastic or non-reversible deformation of materials occurs immediately after a regime of small and completely recoverable elastic deformations, and is governed by the nucleation and motion of defects in the crystal lattice. The motion of these defects transports plastic deformation in discrete packages through the material, and causes the shearing of the crystal lattice. The interaction of dislocations with itself and other defects has been in the focus of materials scientists for an extended time, and is the key in understanding how materials deform at a very fundamental level. In experimental studies, researchers often rely on indirect techniques to investigate the creation and interaction of defects. Most analytical theories of dislocations were developed based on continuum theory and has been extremely successful. Atomistic simulations allow a very detailed view of the defect dynamics. In many studies using molecular dynamics (MD), only specific parts of dislocation mechanics were treated within a simulation (e.g. dislocation nucleation from cracks or dislocation cutting processes). This can mostly be attributed to the size and time scale limitations of the MD. However, with the advent of teraflop computers, scientists are in a situation that billions of atoms can be treated in simulations spanning time scales of nanoseconds, while approaching micrometer length scales. Here we analyze a one billion atom simulation of work hardening in a Lennard-Jones crystal carried out earlier on the world's fastest ASCII WHITE computer. Upon application of loading, two virgin cracks serve as fertile sources for thousands of dislocations on two primary slip planes. These dislocations interact in a very complex way at later stages, and form a complicated topology. In this paper we show that there exist three mechanisms of interactions between the dislocations. These are (1) dislocation cutting processes, with jog formation and subsequent point defect generation, (2) formation of sessile Lomer-Cottrell locks and (3) activation of secondary slip systems by cross-slip and Frank Read mechanisms. Eventually, a steady-state rigid structure of

vacancy tubes, sessile dislocation locks and glissile partial dislocations develops. We analyze and describe this final structure, and show full atomistic details of fundamental mechanisms of hardening. We further present a preliminary statistical analysis of the different defects and its dynamical evolution. This is the first time that such rich set of fundamental phenomena are being seen within a single computer simulation from an ab initio perspective. The analysis underlines the power of continuum mechanics theories in predicting the properties and interactions of topological defects in lattices, as most of the observed effects were predicted by the classical theories. Our results could potentially be used in education, as they provide atomistic animations of dislocation mechanics as they appear in textbooks.

P8.3

Nonuniformity of deformation in nanocrystalline materials. Vitaly Shpeizman and Nina Peschanskaya; Solid State Physics, Ioffe Physicotechnical Institute, Russian Academy of Sciences, St. Petersburg, Russian Federation.

The well-known nonuniformity of deformation in various materials observed both in a multitude of micro- and macroscopic studies is caused by heterogeneity of the material structure and by nonuniformity of the deformation process itself. Modern high-resolution methods of strain and strain rate measurements make it possible to reveal the variations of strain rate on the base of very small increments. The interferometric method used in this work allows to record creep curves and to measure creep rates through each 0.15 micron changes in the length of a sample with an error of less than 5%. In our previous works on polymers we have shown that creep curves consist of repeated sections with relatively high and low velocities and that the period in these strain rate oscillations corresponds to the length of small-scale microfibrils. In the present work we have studied aluminium, copper and other metals with various grain sizes. Special attention was paid to materials with grain sizes 0.5-1 micron that were obtained by multiple equichannel angular pressing (ECAP). Microplastic deformation was observed in all materials at very small stresses which were sometimes less than 10% yield points, but in metals after ECAP the strain rate was ten and more times lower in compare with large grain metals and with single crystals. Two periods of strain rate oscillations in coarse-grain metals were found. One of them was close to the grain size and remained constant with deformation, and the second period was considerably lower than the grain size and decreased with deformation. By contrast, the only period in ECAP metals was more or equal to a mean grain size value and changed slightly with deformation. The model of deformation was suggested which connected the period of strain rate oscillations with characteristic sizes determined by initial structure or by conditions of deformation. Usually, the grain size and the distance between any obstacles on the way of dislocations (impurity atoms, crossing of slip planes, etc) are taken into account as a characteristic structure sizes for deformation in crystals. It follows from our results that the free movement of dislocations through a whole grain or grain boundary deformation is an elementary deformation act for ECAP metals, sometimes only the largest grains from grain-size distribution being involved in an initial stage of deformation. By measuring the period of strain rate oscillations we can follow the grain size evolution at different stages of deformation or after any thermal and mechanical treatment of ECAP metals.

P8.4

Calculation of X-ray diffraction patterns for computer generated nanocrystalline systems. Peter Michael Derlet, Zeljka Budrovic and Helena Van Swygenhoven; Paul Scherrer Institute, PSI-Villigen, Switzerland.

The calculation of two-theta X-ray diffraction profiles for multi-million atom computer generated nanocrystalline Ni systems is presented for a variety of different grain sizes. Peak profile analysis is performed using a standard Warren-Averbach analysis. The derived mean grain size and root-mean-square inhomogeneous strain quantities are compared to similar quantities obtained by direct structural investigation and visualisation of the nc atomic configurations. Debye-Waller factors are also calculated from the theoretical X-ray spectra and compare well with those derived from the phonon properties of the nc system. Theoretical X-ray spectra derived from nc-samples which are mechanically deformed via application of a uni-axial tensile stress are also presented.

P8.5

Compressive Behavior and Deformation Mechanisms of Cryomilled Nanostructured Al-Mg alloys. Guojiang Fan, Y. S. Park, B. Q. Han and E. J. Lavernia; Chemical Engineering and Materials Science, University of California, Davis, California.

The low tensile ductility that is frequently reported for nanostructured alloys that are processed via a milling (e.g., attrition, cryomilling, etc) and consolidation is believed to be due to a lack of

dislocation activity. In contrast, extensive plasticity is commonly observed in many nanostructured materials during compression. In an effort to provide insight into this seemingly contradictory behavior, the present study was undertaken. Cryomilled Al-Mg alloys were used, and compression testing was completed on samples that were polished to a mirror finish in order to facilitate microstructural analysis. The effect of strain rate and strain level on the morphology of the deformed area as well as stress-strain relationships were analyzed. The deformation mechanisms in terms of the interplay between dislocation slip and shear banding are discussed.

P8.6

Mechanically-Milled Nanocrystalline Powders of Equiatomic Fe-Ni and Fe-Co. Ian Baker, May Hourani, Markus Wittmann and Basavaraju Shashishekar; Thayer School of Engineering, Dartmouth College, Hanover, New Hampshire.

Nanocrystalline powders of both Fe-Ni and Fe-Co were produced by mechanical alloying equiatomic amounts of the elemental powders using a high-energy ball mill. In addition, mechanical milling was performed on powders of stoichiometric FeCo filed from a casting. The microstructural evolution was studied as a function of both milling time and subsequent annealing using X-ray diffractometry, scanning electron microscopy and differential scanning calorimetry. The magnetic behavior of the powders was characterized using both a vibrating sample magnetometer and a magnetic force microscope. For FeCo produced from elemental powders, a reduction in grain size coupled with an increase in coercivity was observed as function of milling time, whereas the milled stoichiometric FeCo showed a peak in coercivity at a grain size of 50-100nm, a feature noted by others in a number of other soft magnetic alloys. The phases present after milling Fe-Ni and their effects on the magnetic properties will also be discussed. This research was supported by NIST grant 60NANB2D0120.

P8.7

In-situ Observations of Strain due to Phase Transformation of Pb Inclusions in Al. Lihua Zhang¹, Erik Johnson² and Uli Dahmen¹; ¹National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, California; ²Niels Bohr Institute, University of Copenhagen, and Department of Materials Research, RISØ National Laboratory, Copenhagen, Denmark.

The appearance and decay of strain contrast around faceted Pb inclusions embedded in an Al matrix during solidification of the inclusions have been observed by in-situ transmission electron microscopy (TEM). The strain is due to a 3% volume decrease of the Pb inclusions upon solidification. In the present work, in-situ microscopy was used in the temperature range between 180° and 350° to observe the process of melting and solidification of Pb and Pb-alloy inclusions with different sizes and compositions. The magnitude of the elastic strain was determined from observations of the strain lobes surrounding the inclusions using two-beam conditions, and the decay of strain with time was analyzed in detail from video recordings depicting the gradual disappearance of the strain lobes. For small particles, the volume change upon transformation is initially accommodated elastically while larger particles are found to generate dislocations via climb or loop punching. The experiments indicate that the decay time of the strain lobes depends on temperature, foil thickness, and size of the inclusions. The decay of the elastic strain field with time is thought to be controlled by the supply and mobility of lattice vacancies around inclusions. By using different alloy inclusions with different solidification temperatures, it was possible to observe the process at different temperatures and thus obtain the activation energy and confirm the mechanism. The rate of decay was found to be consistent with earlier observations on dislocation loop annealing in quenched alloys. This work was supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, and the Danish Natural Sciences Research Council.

P8.8

Stress Distribution in Ultra Thin SiO₂ Film/Si Substrate System Measured by a Low Level Birefringence Detection Technique. X. H. Liu¹, H. J. Peng¹, S. P. Wong¹, Shouan Zhao² and J. B. Xu¹; ¹Electronic Engineering Department, Chinese University of Hong Kong, Hong Kong, China; ²Applied Physics Department, South China University of Technology, Guang Zhou, Guangdong, China.

In this work, a low level birefringence detection system was employed to study the stress distribution in Si substrate induced by thermally grown ultra-thin SiO₂ film. According to traditional bi-metallic strip theory, it is expected that the stress should show a linear dependence on depth with the zero stress point located at the position of two third of the thickness of the substrate from the SiO₂/Si interface. The

linear dependence on depth was verified but the position of the zero stress point was found dependent on the thickness of SiO₂ film and the oxidation conditions. The zero stress point seemed to move towards the bottom of the Si substrate as the thickness of the SiO₂ film became thinner. Moreover, it happened that no zero stress point was observed in the Si substrate when the SiO₂ films became sufficiently thin (e.g. 20 nm). To explain the experimental results, we propose to associate this phenomenon with point defect injection during the oxidation process. Our model also suggests that information about point defect injection during thin oxide growth can be obtained by this high sensitivity measurement of stress distribution in the Si substrate. This work is supported in part by the Research Grants Council of Hong Kong SAR (ref. no. CUHK4370/02E).

PS.9

Bending of Copper Thin Single Crystals. Masao Doyama, Yoshiaki Kogure, Tadatoshi Nozaki and Yukie Kato; Materials, Teikyo University of Science and Technology, Uenohara, Yamanashi, Japan.

Copper single crystals of thin films were bent. Molecular dynamics were used with an embedded atom potential. It was found that the old model of bending is wrong. Macrobending and atomic or micro-bending should be distinguished. Macro-bending without containing dislocations is possible. These can be distinguished by X-ray Laue patterns. It was found that dislocations were quite difficult to be initiated on a very smooth flat surface under tension. It is also difficult to initiate dislocations by pure bending, if the surface is atomically smooth. It is easy to initiate dislocations at the wrinkles of slip plans under compression. When a notch is present on a surface, dislocations are created near the tip of the notch. Single crystals suddenly became polycrystals under severe pure bending, even at low temperatures. In copper crystals, partial dislocations were always created leaving stacking faults on one side. Formation of dislocations as a function of film thickness is also presented.

PS.10

Unconfined Twist: a Simple Method to Prepare Nanocrystalline Materials. Yonghao Zhao, Xiaozhou Liao and Yuntian Zhu; Materials Science and Technology, Los Alamos National Lab., Los Alamos, New Mexico.

Severe plastic deformation (SPD) is a promising method to prepare bulk nanocrystalline materials. In our work, a new simple SPD method - unconfined twist was employed to prepare nanocrystalline Fe wire. The coarse grained Fe wire was fixed at both ends, and was twisted from one end. The deformation strain can reach as much as 5.0. The twisted sample was composed of both equiaxial crystallites (about 100 nm) and lamellar crystallites (about 100 nm width). The yield stress and microhardness increase about 1 time compared with those of the unprocessed sample. The formation mechanism of nanostructure during twisting will be discussed.

PS.11

Abstract Withdrawn

PS.12

A new mechanism for the negative strain rate sensitivity of solid solutions. Catalin Picu, Rensselaer Polytechnic Institute, Troy, New York.

A new mechanism leading to negative strain rate sensitivity and the Portevin-LeChatelier effect in dilute solid solutions is presented. Although the mechanism is general, the Al-Mg system is used for exemplification. It is shown by means of atomistic simulations that, in this system, both bulk and pipe diffusion are too slow and cannot be used in conjunction with the classical mechanism of dynamic strain ageing to explain the macroscopic material behavior. The mechanism proposed here is based on the effect of solute clustering on the strength of dislocation junctions. A dislocation dynamics model that captures the mechanism is developed. The model parameters are calibrated for the Al-Mg system based on atomistic simulations. The model predictions are discussed against the predictions of the classical mechanism and in conjunction with experimental observations.

PS.13

ECAP Processing of Bulk Nanostructured Copper Using FEM Studies. Vladimir S. Zherakov, Igor N. Budilov, Igor V. Alexandrov and Ruslan Z. Valiev; Ufa State Aviation Technical University, Ufa, Russian Federation.

Processing of bulk nanostructured metals by equal-channel angular pressing (ECAP) exemplifies a multi-factor experiment, because its result is influenced by both the structure of initial materials, tool design and processing parameters. In this connection, application of computer simulation can be very useful for such processing. In this paper we report the results of the analysis of processes under way during ECAP of a copper billet. The finite-element method (FEM) by

LS-DYNA and Superform codes has been applied in this work. 3D analysis has revealed that in the area of contact interaction between the billet and the die-set the plastic flow grows very heterogeneous. The influence of the main processing parameters on the billet stress-strain state and a tool load has been investigated. Recommendation on a die-set design for ECAP of ultrafine-grained copper billets with different dimensions have been elaborated.

PS.14

Texture and Microstructure evolution in Silver and Aluminum Thin films with FACET. Asit Rairkar and James B Adams; Science & Engineering of Materials Ph.D. program, Arizona State University, Tempe, Arizona.

Metallic polycrystalline thin films are used in a plethora of applications, including especially metallic interconnects for the microelectronics industry. Despite the numerous approaches at modeling and simulating processing of these films, there have not been many simulation tools, which can accurately predict texture and microstructure evolution in these films. We have developed a novel 2D model called FACET for the simulation of polycrystalline thin film growth on a micron scale at realistic deposition rates. The basic idea is to use the results of smaller-scale atomic simulations (density functional theory, molecular dynamics, and lattice Monte Carlo) to provide input and guidance on the evolution of grain structure and texture on a micron scale. The feature scale model is based on describing grains in terms of two-dimensional faceted surfaces and grain boundaries. The model includes the major phenomena involved in film growth, including deposition, nucleation, surface diffusion (on the substrate and on the growing film), inter-facet diffusion, and grain growth and coarsening. In addition, the texture of each grain is treated individually, so that the texture evolution of the system can be simulated. We attempt to validate our FACET code with previous experimental work in Ag and Al films by presenting qualitative and quantitative comparisons of texture and microstructure data. It is well known that fcc films develop a strong <111> texture during growth and especially annealing. However, the exact driving mechanisms for these texture developments have not been fully understood. This paper will also report the results of high temperature Molecular dynamics simulations using EAM potentials to understand mechanisms of texturing and grain coarsening in Aluminum films, which provides insight into various surface energy driven mechanisms for the formation of such strong <111> textures in fcc films.

PS.15

Understanding on Deformation and Failure of Bimodal Nanostructured Materials. Riqing Ye¹, Bingqiang Han¹ and Enrique J. Lavernia¹; ¹Chem.Eng.&Mater.Sci., University of California, Davis, Davis, California; ²Chem.Eng.&Mater.Sci., University of California, Davis, Davis, California; ³Chem.Eng.&Mater.Sci., University of California, Davis, Davis, California.

Available experimental and theoretical studies attribute the low ductility of nanostructured materials to the deficit of dislocation activity. The present study aims to provide insight into a recently proposed hypothesis that one can promote dislocation activity, without a significant loss in strength, by attaining a microstructure that contains multiple length scales, that is from tens of nanometers to hundreds of nanometers. This concept has been successfully demonstrated recently in cryomilled Al alloys containing a bimodal microstructure by experimental results. In the present work, the tensile deformation behavior and failure mode of cryomilled nanostructured aluminum alloys with a bimodal structure are simulated via a unit-cell model under uniaxial tensile loading. The elastic-plastic behavior and the dynamic fracture process of bimodal materials were approximated by Ramberg-Osgood formula and finite element method, respectively. The computer simulation result is found to be in a reasonable agreement with tensile experimental data. It further indicates that the cryomilled aluminum alloys processed with an optimized un-milled coarse grains fraction will have an improved ductility without much sacrifice of strength. The deformation characteristics of bimodal nanostructured materials will also be explored in terms of dislocation mechanisms.

PS.16

Modeling the Stress Evolution of Ion Beam Synthesized Nanocrystals. D O Yi^{1,2}, I D Sharp^{2,3}, Q Xu^{2,3}, C Y Liao^{2,3}, J W Ager², J W Beaman², Z Liliental-Weber², K M Yu², D Zakharov², E E Haller^{2,3} and D C Chrzan^{2,3}; ¹Applied Science and Technology Graduate Group, University of California, Berkeley, Berkeley, California; ²Materials Sciences Division, Lawrence Berkeley National Lab, Berkeley, California; ³Materials Science and Engineering, University of California, Berkeley, Berkeley, California.

Under certain conditions, homogeneous nucleation and growth can lead to substantial stresses in nanocrystals embedded in a host

matrix. In general, stresses can arise from two effects. 1) The matrix/nanocrystal interface tension may place the nanocrystals in a compressive stress state (which is different from the stress state of nanocrystals liberated from their host matrix), and 2) the cavity in the matrix cannot expand sufficiently fast to accommodate the growth of the embedded nanocrystals. We show that these effects lead to increased compressive stresses of a few GPa, and we present a model for the relaxation of these additional stresses. The model reflects the effects of surface tension, potential phase transformations at or near the processing temperature, and differential thermal expansion. It assumes that the cavity stresses can be relaxed through a diffusive process within the matrix. It is demonstrated that the model describes well the stress evolution of ion beam synthesized Ge nanocrystals embedded in a silica matrix. This work is supported by the Directorate, Office of Energy Sciences, Office of Basic Energy Sciences, of the Department of Energy under contract No. DE-AC03-76SF00098.

P8.17

Atomistic Simulation of Dislocation Interaction with a $\Sigma=5$ (210) Grain Boundary During Nanoindentation of Ni.

Ho Jang¹ and Diana Farkas²; ¹Department of Materials Science and Engineering, Korea University, Seoul, South Korea; ²Department of Materials Science and Engineering, Virginia Polytechnic Institute, Blacksburg, Virginia.

Molecular dynamics simulation of nanoindentation was performed using embedded atom potentials. The indentation was simulated on a Ni substrate using a diamond indenter. In this study, we focused on the indentation of a $\Sigma=5$ (210) grain boundary with the dislocations that were nucleated and expanded as loops in the course of nanoindentation. The grain boundary was located in the middle of the substrate and was perpendicular to the indentation direction. Results showed that the dislocation loops propagated on {111} slip planes as pairs of Shockley partials accompanying stacking faults approximately 7 atomic distances wide. The dislocations changed grain boundary structure as they merged into the grain boundary, displacing grain boundary atoms according to the Burgers vector of the lattice dislocations. Detailed analysis of atom displacements at the grain boundary suggested that the local force was built up on the atoms that were displaced by the dislocations across the grain boundary. The effect of the grain boundary on the indentation was also examined by simulating nanoindentation using Ni substrates with and without a grain boundary. Results showed that the presence of a grain boundary strongly affect the indenting speed and dislocation motion during nanoindentation.

P8.18

Analysis of Residual Stress and Damage Durability with Thermal Fatigue Behavior in Thermal Barrier Coatings.

Dong-Ho Park¹, Hyung-Jun Jang¹, Yeon-Gil Jung¹, Jung-Chel Chang² and Ungyu Paik³; ¹Dept. of Ceramic Science and Engineering, Changwon National University, Changwon, Kyungnam, South Korea; ²Power Generation Lab, Korea Electric Power Research Institute, Daejeon, South Korea; ³Dept. of Ceramic Engineering, Hanyang University, Seoul, South Korea.

The advanced multi-layered ceramic coatings applied on metallic substrates are generally used as thermal barrier coatings (TBCs) in gas turbine components and diesel engines. Demands for improving performance of these turbine and engines are met in part by increasing and decreasing the combustion and cooling temperatures, respectively. However, Increase of the temperature difference within the turbine and engines leads to the service limits of current TBCs and superalloys. Therefore, the estimation and understanding of properties of TBCs, such as thermal behavior, residual stress, and damage tolerance, are essential for improving the reliability and lifetime of TBCs. Herein, we describe the analysis of residual stress and damage durability with thermal fatigue behavior in TBCs. For which TBCs were fabricated with two kinds methods of APS and HVOF. Damage durability was observed with thickness of coating and bonding layers, and compared to each other with fabrication methods. Mechanical properties of hardness and elastic modulus were investigated using nano-indentation with thickness of coating and bonding layers at different thermal fatigue conditions. Also, the critical loads for yielding (P_Y) and cracking (P_C) were determined through Hertzian indentation, including the stress-strain behavior of each layer and condition. The effects of thickness of coating and bonding layers with fabrication method on the residual stress and damage durability of TBCs are investigated extensively.

P8.19

Stress-diffusion coupling: extending continuum mechanics to the defect scale. Mathieu Bouville¹, Michael L. Falk¹ and Krishna Garikipati²; ¹Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan; ²Mechanical Engineering, University of Michigan, Ann Arbor, Michigan.

Nanostructured materials, particularly those grown via heteroepitaxy, often exhibit large residual stresses due to lattice mismatch. These stresses can have a significant effect on the stability of structures and dopant profiles by altering diffusivities and by introducing gradients in the chemical potential. In addition, quantifying the stress fields of defects is important for calculating the formation free energies of activated complexes that mediate dopant diffusion. We examine the stress field in the vicinity of point defects in silicon in order to determine (i) the scale at which continuum theories can adequately model the stress field and (ii) numerical techniques that can be used to accurately extract thermodynamic quantities such as the formation volume that relate the local stress to the chemical potential via the formation enthalpy. We discuss how the elasticity formulation of a center of contraction can be used to analyze atomistic data.

P8.20

The Defects as the Objects of Selforganization of the Crystal Structure, Subjected to External Deformation Influence.

Mikhail D. Starostenkov and Gennady M. Poletaev; General Physics Department, Altai State Technical University, Barnaul, Russian Federation.

Structure-energetical transformations in the initially ideal crystal, as open system, subjected to external deformational influence are studied in the present paper. The research was made by the method of computer simulation. The research is concerned with the crystal of solid Al with FCC lattice. The interactions between different pairs of atoms in the crystal are described by semiempirical Lennard-Jones potential taking into account the bonds of the atoms in the first seven coordinational spheres. The given potential is chosen because Koshi relation is well satisfied for the crystals of inert gases at low temperatures. The crystal was presented by the calculated block, consisting of 30*100 of one-dimensional chains of atoms. The chains were displaced as a whole in the direction perpendicular to the calculated block. The atoms were allowed to displace arbitrarily in the plane of the calculated block. The minimum of internal energy of the calculated crystal block was determined by the method of variational quasistatics at various displacements of atoms in the plane of the block and along atomic chains. The crystal structure repeated under the influence of periodical boundary conditions outside the calculated block. Small heating of the crystal, given by the distribution of the velocities of the atomic displacements (Boltzman statistics) was made for the realization of the process of structure relaxation. Impulse loading of the crystal, simulating deformation of shift compression, tension and combination of shift and compression was given after the relaxation of the structure of the ideal crystal packing. In the result, the peculiarities of the sequence of elastic, plastic deformation and fracture of the material in the initially perfect state of crystal were determined. It was found 12 stages of structure-energetical transformation. It was shown, that the definite state of non-linear unstability of the crystal appeared at any type of loading between different stages. Then self-organised defect structures in the material formed as the reaction on this state.

P8.22

The Effects of Internal Variables on Interfacial Debond Strength of Cu/Ta/SiO₂/Si Multilayers Measured by Nanoscratch Test.

Atsuko Sekiguchi and Junichi Koike; Dept. of Materials Science, Tohoku University, Sendai 980-8579, Japan.

Nanoscratch test has been used to measure the debond strength of heterophase interfaces. However, the measured strength often exhibits a large data scatter, giving a false impression that the nanoscratch test is not a reliable nor accurate method. Recently, we reported that the nanoscratch test measures adhesion strength in a nanometer spatial resolution. Because of this high resolution, the measured data were expected to change depending on the spatial variation of microstructure, such as crystallographic orientation and structure of the grains meeting at the interface, as well as other internal variables. In this work, we attempted to understand quantitatively the effects of internal variables on the adhesion strength by calculating stress distribution in a multilayer stack of Cu/Ta/SiO₂/Si using a finite element computer code. Investigated variables were residual stress and elastic/plastic anisotropy in the Cu film. Stress distribution was calculated by using an actual geometry of nanoscratch test with a 1 μ m conical diamond indenter driven to a certain depth of the Cu layer at the time of interface failure. Plasticity of the Cu layer was found to induce a strain-compatibility effect at the Cu/Ta interface, giving rise to a large stress concentration of tension and shear. The spatial range of the stress concentration was in the order of 50 to 100 nm. The magnitude of stress concentration increased with increasing the compatibility effect by making Cu softer or by decreasing scratch speed to allow Cu to plastically relax. Stress concentration also increased with decreasing compressive residual stress or with increasing tensile residual stress. The larger the stress concentration is

at the interface, the less scratch force is required to debond the interface. Thus, determination of internal variables and stress calculation was found to be essential in the evaluation of intrinsic debond strength of the interface. The calculated results will be compared with experimental data reported elsewhere and a good correlation will be shown.

P8.23

How Much Can Surface Roughness Influence Nanoindentation Tests? - Nanoindentation Tests of Rough Surfaces with a Flat Indenter Tip. Wei-Hua Xu, Jianrong Li and Tong-Yi Zhang; Department of Mechanical Engineering, Hong Kong University of Science and Technology, Hong Kong, Hong Kong.

Elastic-plastic contacts of rough surfaces were investigated by conducting nanoindentation tests on Polymethylmethacrylate (PMMA) using a flat tip (1 micrometer x 20 micrometer). During an indentation test with a flat punch, the overall deformation can be divided as the bulk deformation and the surface deformation. Under small loads, the rough surface layer deforms elastic-plastically, while the bulk deforms elastically. An elastic-plastic bearing ratio model was proposed based on the PW theory (Pullen and Williamson, 1972). Two-dimensional finite element analyses were also conducted. Good agreement was found between the theoretical predictions, experimental results, and finite element simulations, which indicates that the surface roughness plays an important role during the nanoindentation test.

P8.24

Stress Reduction in Sputter Deposited Thin Films Using Physically Self-Assembled Nanostructures as Compliant Layers. Tansel Karabacak, Jay J Senkevich, Gwo-Ching Wang and Toh-Ming Lu; Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, New York.

The stress in thin films has been a major limiting factor for obtaining high quality films. We will present a new strategy of stress reduction in sputter deposited films by a nano-compliant layer at the substrate using physically self-assembled nanostructures obtained either by an oblique angle deposition technique^{1,2} or by a high working-gas pressure process prior to the deposition of the continuous film. The technique is all in-situ, does not require any lithography steps, and the nanostructures are made of the same material as the deposited thin film. The nanostructures have a lower material density and can act as a compliant layer to reduce the stress of the later deposited continuous film. By using this approach we were able to reduce stress values by approximately one order of magnitude in sputter deposited tungsten films. Our experimental results agree well with the predictions of a theoretical model that we developed to explain the stress relief through the nanostructured compliant layer. In addition, these lower stress thin films exhibit a stronger adhesion to the substrate and the delamination is avoided. This strategy leads to the growth of much thicker films with high structural reliability. ¹Y.-P. Zhao, D.-X. Ye, G.-C. Wang, and T.-M. Lu, "Novel nano-column and nano-flower arrays by glancing angle deposition", Nano Letters 2, 351-354 (2002). ²K. Robbie, M. J. Brett, and A. Lakhtakia, "Chiral sculptured thin films," Nature 384, 616-616 (1996).

P8.25

A new technique for the evaluation of the elastic modulus with straight sided buckle in the nano-scaled thin compressive film on the patterned substrate.

Myoung-Woon Moon¹, Tae-Young Kim^{1,2}, Kwang-Ryeol Lee² and Kyu Hwan Oh¹; ¹School of Materials Science and Engineering, Seoul National University, Seoul, South Korea; ²Future Technology Research Division, KIST, Seoul, South Korea.

A method for exact measurement of the elastic modulus in diamond-like carbon (DLC) films of the thickness of 40-200nm was suggested by using the analysis of straight sided buckle on patterned substrate. It was shown that a straight sided buckle can be introduced even in equi-biaxial stress state by controlling the buckling width of the pattern. The sinusoidal profile of buckle such as the amplitude and the width, being characterized by an atomic force microscope (AFM), would be dependent on the elastic modulus and the residual stress of the thin film. Mechanical properties of two different DLC films, i.e. hydrogenated amorphous carbon (a-C:H) film deposited by r.f.-PACVD and tetrahedral amorphous carbon (ta-C) films prepared by filtered vacuum arc process, were estimated by using this technique. The elastic modulus of the films were estimated to be 87-100 GPa for a-C:H and 450-550GPa for ta-C films. These values are comparable to those obtained by the nano-indentation method.

P8.26

Synthesis and Characterization of Fe-Co Nanocrystalline Alloys. Mohammad Mujahid and Jie Zhu; Materials Engineering, Nanyang Technological University, Singapore, Singapore.

Nanostructured alloys have great potential as soft magnetic materials. In particular, nanocrystalline Fe-Co and Fe-Co-Ni based alloys are believed to be good candidates for imparting improved magnetic behavior in terms of higher permeability, lower coercivity, reduced hysteresis loss and higher Curie temperatures. In the present work, various compositions of Fe-Co and Fe-Co-Ni alloys have been prepared using mechanical alloying (MA) in a planetary ball mill under controlled environment. The influence of milling parameters (such as milling time and ball-to-powder ratio) on the crystallinity and crystal size in the alloys has been studied. The particle size and morphology of MA powders was also investigated using scanning electron microscopy. In addition, pressure less sintering was employed for consolidation of the MA powders. The crystal size and internal strain in both the MA powders as well as compacted samples was measured using X-ray diffraction. It has been shown that the crystal size could be reduced down to less than 15 nm in these alloys. The nanocrystalline materials thus obtained were also evaluated for magnetic behavior, i.e. coercivity and saturation magnetization. Finally, the influence of grain size and internal strain on the magnetic properties has been discussed.

P8.27

Microstructure Refinement in Single-Phase Solid Solutions by Machining. Srinivasan Swaminathan¹, Srinivasan Chandrasekar¹, W Dale Compton¹ and Kevin P Trumble²; ¹School of Industrial Engineering, Center for Materials Processing and Tribology, West Lafayette, Indiana; ²School of Materials Engineering, Center for Materials Processing and Tribology, West Lafayette, Indiana.

It is well known that significant microstructure refinement can be realized by subjecting materials to large strain deformation. One method of realizing very large plastic strains in a single stage of deformation is by the process of chip formation in machining. It has been demonstrated that ultra-fine grained, including nanostructured, materials can be created in a variety of metals and alloys by this process. A study has been made of microstructure refinement in single-phase solid solutions, especially that arising from solute-related effects. Chips were produced by machining dilute copper solid solutions containing equal atomic percentages of different solutes. The solutes were chosen specifically for their influences on the stacking fault energy (SFE) of copper. Different levels of strain and temperature were introduced into the material during chip formation by careful selection of machining parameters. The microstructure, hardness and annealing behavior of the chips were characterized as a function of the deformation conditions and SFE. Correlations are established between the nanocrystalline microstructure of the chip, and the deformation parameters and SFE. Implications of the machining approach to study microstructure refinement, and large volume creation of ultra-fine grained materials will be discussed.

P8.28

Role of deformable fine spinel particles in high-strain-rate superplastic flow of tetragonal ZrO₂. Koji Morita, Keijiro Hiraga, Byung-Nam Kim and Sakka Yoshio; National Institute for Materials Science, Tsukuba, Ibaraki, Japan.

High-strain-rate superplastic flow is attained in tetragonal ZrO₂ dispersed with fine MgAl₂O₄ spinel particles, where tensile ductility exceeds $\approx 250\%$ at 1823 K and at an initial strain rate of $\approx 0.7 \text{ s}^{-1}$. The fine spinel dispersion can improve strain rate more than 10^3 times as compared with monolithic tetragonal ZrO₂. The high-strain-rate superplastically deformed ZrO₂-spinel composite reveals an interesting microstructural feature. In the most superplastic ceramics, grains retain their initial equiaxed shape even after large deformation, whereas for the ZrO₂-spinel composite, the dispersed spinel particles highly elongate along tensile direction after deformation. TEM observation reveals activated dislocation motion within the elongated spinel particles though the flow stress is 10-15 times smaller than the yield stresses of spinel single crystals. This suggests that significant stresses higher than flow stresses should be generated in the ZrO₂-spinel composite during superplastic flow. The flow behavior can be characterized by a stress exponent of ≈ 2.0 so that grain boundary sliding (GBS) can generally be considered as the predominant flow mechanism. The deformation is controlled by the rate of accommodation process of stress concentrations around multiple grain junctions exerted by the predominant GBS mechanism. The dislocation motion activated within the elongated spinel particles suggests that, in the present material, the stress concentrations can be relaxed through the deformation of the fine spinel particles. Thus, the enhanced accommodation due to the deformable spinel particles makes it possible to attain the high-strain-rate superplastic flow in tetragonal ZrO₂.

P8.29

Point defect dynamics in Vanadium(alloys). Joerg G Rottler and David J Srolovitz; Princeton Materials Institute, Princeton, New

Jersey.

Point defects are created in abundance in metals under irradiation conditions and determine the evolution of their mechanical properties on large time scales, in particular radiation swelling. We use classical molecular dynamics (MD) and kinetic Monte Carlo (kMC) methods to investigate the dynamics of self-interstitials and vacancy defects in Vanadium and its alloys, which are prime candidates for use in fusion reactor environments. In V, self-interstitial motion is characterized by an extremely fast one-dimensional diffusion along the crystallographic [111] axes, with occasional directional changes occurring through rotations. MD simulations show that the temperature dependence of this diffusion process is highly non-Arrhenius. Vacancy diffusion takes place on a much slower time scale and leads to their accumulation into voids. In order to access larger length and time scales, a kMC model is parametrized with the diffusivities measured in MD. We discuss the evolution of the void cluster size distribution and swelling rates and also compare our results to classical mean-field rate equations.

P8.30

Molecular Dynamics of Cross-Slip in Copper. Dan Mordehai¹, Itzhak Kelson¹ and Guy Makov²; ¹Tel Aviv University, Tel Aviv, Israel; ²Department of Physics, NRCN, P.O. Box 9001, Be'er Sheva, Israel.

The presence of dislocations constitutes one of the basic building blocks of any theory of plasticity, and has been studied for many years both experimentally and theoretically. Yet, in the developing study of nanoscale structures and materials, the size of the system complicates the analysis. The behavior of system with nanoscale structures can no longer be studied using macroscopic models (e.g. the validity of the Hall-Petch equation for a material with nanoscale grains). While the contribution of dislocation pile-ups and clusters of dislocations can be neglected in this size regime, the interaction between dislocations plays a significant role. Such small scale and dynamic processes are not observable in experiments. Using molecular dynamics methods we study the cross-slip mechanism in Cu as a function of both temperature and stress. Both straight and flexible dislocations were considered. Spontaneous annihilation via the cross slip mechanism was observed for short separation distances between the dislocations. At larger separations annihilation didn't occur when no stress was applied and a bound metastable state was found for the two dislocations. Annihilation from this metastable state was induced by increasing the temperature or applying an external stress, which decreased the dissociation width of the screw dislocations. The activation energy and volume of the cross slip process are presented.

P8.31

Microstructure and Mechanical properties of Rapidly Solidified and Extruded Mg-Zn Alloys. George Levi^{2,3} and Dan Shechtman³; ¹Metallurgy Division, National Institute of Standards and Technology, Gaithersburg, Maryland; ²Materials Science and Engineering Laboratory, National Institute of Standards and Technology, Gaithersburg, Maryland; ³Materials Engineering, Technion-Israel Institute of Technology, Haifa, Israel.

Mg alloys have found numerous practical applications, mainly thanks to their high strength to weight ratio. However, these applications are often limited by the relatively low strength of these alloys as compared to other competing materials such as aluminum alloys. Therefore, a lot of effort has been dedicated to developing technologies capable of producing Mg alloys with improved mechanical properties. In this study we correlate the microstructure and relatively high mechanical strength of an Mg-Zn alloy that contains small additions of Zr, Y and Ce. The alloy was produced by rapid solidification of ribbons followed by combination, compaction and extrusion. The study is aimed at understanding mechanisms that control and affect the strength of these alloys. A detailed micro structural investigation was conducted, by optical microscopy (OM), X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM), combined with electron dispersive spectroscopy (EDS). TEM studies of the extrusions revealed fine, submicron to micron size microstructural features, consisting of equiaxed Mg grains having small amounts of the alloying elements in solution. TEM also revealed nano-sized precipitates residing within the Mg grains, and nano- or submicron-sized precipitates residing at the Mg grain boundaries. Both the intra- and the inter-granular precipitates contribute to the strength of the alloy. Their structure and chemistry, as well as their relationship to other microstructural features were investigated, too. It was also found that the alloy phase compositions, prior to, and after the extrusion, are significantly different.

P8.32

Fracture Toughness and Tensile Properties of an Oxide Dispersion-Strengthened Ferritic Steel. Mikhail A. Sokolov, David Hoelzer and Roger Stoller; ORNL, Oak Ridge, Tennessee.

The reduced-activation ferritic-martensitic (RAFM) steels are the primary candidates for a fusion power plant first wall and blanket structure. The ferritic-martensitic steels are known to resist radiation swelling and have good thermal conductivity. However, their utilization is limited to around 600°C due to inferior tensile and creep strength at higher temperatures. One way to increase the temperature capabilities of RAFM steels is by incorporation of an oxide dispersion. Elevated temperature strength in these steels is obtained by a high number density of ultra-fine, nanometer-scale yttria-titanium-oxygen complex particles dispersed in a ferritic matrix. The oxide dispersion-strengthened (ODS) steels are being developed and investigated for fission and fusion application in Japan, Europe, and the United States. In this paper, the fracture toughness and tensile properties of an ODS steel with nominal composition of Fe-12Cr-2.5W-0.4Ti-0.25Y2O3 (designated 12YWT) were investigated and compared to commercial RAFM steels. For 12YWT steel, particles were estimated to be only few nm in diameter at a number density of $1-2 \times 10^{23} \text{ m}^{-3}$. Small, 1.6-mm thick and 3.2-mm wide, 3-point bend specimens were used for fracture toughness characterization of this steel. Specimens were fatigue pre-cracked to initial crack length (a) to width (W) ratio of 0.5 and tested quasi-statically in the temperature range from -50°C to 100°C. Specimens tested up to 50°C exhibited elastic-plastic cleavage fracture that was typical for the transition region in ferritic steels. Specimens tested at 100°C exhibited ductile stable crack growth. In these cases, the J-intergal at the onset of stable crack growth (J_{Ic}) was determined from the J-R curves. Their equivalent values in terms of stress intensity, K_{JIC} , were about 100 MPa $\sqrt{\text{m}}$. This study showed that oxide dispersion resulted in significant decreases in the toughness properties compared to commercial RAFM steels, although appreciable level of toughness was still retained. Tensile tests were performed at different temperatures from room temperature to 800°C. As expected, this material exhibited very high yield strength, 1300 MPa, at room temperature. For comparison, yield strength of commercial RAFM steel is about 550 MPa. Yield strength of 12YWT decreases as test temperature increases and at 800°C yield strength is about 323 MPa.

P8.33

Nano-Mechanics of Small-Volume Thermal Spray Deposits on Substrates. Andrew Gouldstone^{1,2}, Li Li^{1,2} and Sanjay Sampath^{1,2}; ¹Department of Materials Science and Engineering, Stony Brook University, Stony Brook, New York; ²Center for Thermal Spray Research, Stony Brook University, Stony Brook, New York.

Nano-crystalline materials are of high technological interest due to their potentially high strength, ductility and toughness. The physics of nano-crystalline deformation is not fully understood, but recent advances in nano-mechanical probes and numerical analyses have driven a growth spurt in its study. Thermal spray, a well-established coating technology, routinely deposits material in the form of small-volume (thickness = 1-3 μm) structures, referred to as *splats*, that exhibit columnar grains of 10-100 nm diameter under certain conditions. In addition, the morphology, phase and residual stresses of splats can be controlled via selection of spray input parameters. At the Center for Thermal Spray Research, we have thus recognized the potential for a systematic nano-mechanical study, and are currently performing mechanical characterization on a wide range of splat materials. In this presentation, we discuss illustrative observations of nano-crystalline structure in splats, and results of nano-indentation experiments on metal and ceramic splat materials. Resulting force-displacement ($P-h$) curves are analyzed in the context of discrete dislocation activity and residual stress, and are compared with results from nano-indentation of well-annealed bulk materials.

P8.34

A Study of Bicrystals using a Dislocation-Based Continuum Model with Inherent Length Scale. Firas Akasheh¹, Athanasios Arsenlis² and Hussein Zbib¹; ¹Washington State University, Pullman, Washington; ²Lawrence Livermore National Laboratory, Livermore, Washington.

A dislocation-based continuum model for the plastic deformation of FCC crystals is developed where dislocation densities are treated as state variables having evolution laws guided by dislocation dynamics (DD) simulations. The dislocation population on each slip system is expressed in terms of a discrete basis consisting of 4 base densities: two edge densities of positive and negative polarities and likewise for the screw dislocations. In this way the crystallographic nature of dislocations is maintained, making the model more realistic. Furthermore, attaching a polarity to densities allows the treatment of the coupled evolution of statistically stored dislocations (SSD) and geometrically necessary dislocations (GND). The evolution of SSDs is governed by the law of conservation of Burgers vector and includes significant dipole generation/annihilation mechanisms, while GNDs evolve through the divergence of density fluxes and certain non-Burgers vector-conserving dislocation-dislocation reactions. The

evolution of the polarity leads to the strain gradients and nonhomogeneous deformation and is related to Nye tensor. The model is implemented using the finite element method and used to study different problems in bicrystals in a simplified 2D plane strain arrangement with double and triple slip. As for the grain boundary, which is known to play a crucial role in the deformation process, the model provides the necessary ingredients to impose the various observed dislocation-grain boundary interactions through the conservation of Burgers vector principle. The study includes the effect of the size and crystals misorientation on the stress-strain response as well as the development of dislocation patterns with the component crystals and around the grain boundary. Results show that length scale arises naturally in this model with imposing it in the constitutive relations.

P8.35

Determination of macroscopic parameters from microstructural simulations: anisotropic sintering.

Michael Braginsky and Veena Tikare; Sandia National Laboratories, Albuquerque, New Mexico.

One of the most important problems in modeling of sintering is the determination of macroscopic properties based on microstructural evolution. The connection between materials science theories of sintering, which study microstructural evolution based on complex diffusion mechanism, and macroscopic continuum sintering models, i.e., plastic or nonlinear-viscous compaction of porous bodies, is currently being established using methods of micromechanics on simplified microstructures. In the current work, we study ways to obtain parameters of macroscopic models based on microstructural simulations. The connection is being made through the free energy, which is in our approach the basis for the determination of microstructural evolution. As the main example, parameters for a viscous macroscopic continuum sintering model - namely, sintering stress and viscous moduli - are calculated based on the kinetic Monte-Carlo simulation of microstructural evolution during sintering. The determination of sintering stress for a compact that deforms isotropically is straightforward: the sintering stress is determined as the derivative of the free energy with respect to volume. The bulk viscous modulus is determined based on sintering stress as the next step. The system becomes significantly more complicated in the case of anisotropic sintering, where the sintering stress is no longer characterized by just a scalar. In that case, the sintering stress can still be defined as the derivative of the free energy, now with respect to the macroscopic strain, but it cannot be determined uniquely based on this definition. The sintering stress has to be determined from the simulations based on the viscous properties, which have to be determined first from the evolution of the dissipative potential. The developed methodology is applicable to a wide range of microstructures at different length scales establishing an important link between mesoscopic mechanisms of sintering and the macroscopic mechanical behavior of the sintered material. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under the Contract DE-AC04-94AL-85000.

P8.36

Effect of Oxygen and Nitrogen Doping on Mechanical Properties of Silicon Using Nano-Indentation.

Abdennaceur Karoui¹, George Rozgonyi¹ and Ted Ciszek²; ¹Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina; ²Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina; ³National Renewable Energy Laboratory, Golden, Colorado.

The effects of O and N on the mechanical properties of nitrogen doped Czochralski (N-CZ) and float zone (N-FZ) silicon have been studied using nano-indentation in order to find the optimum O and N doping levels for material strengthening without scarifying the high lifetime offered by FZ Si. Nano-indentation and load controlled nano-scratch tests have been carried out using the Hysitron Triboindenter. Nitrogen free FZ Si exhibited low hardness of 6.5 GPa and elastic modulus of 104 GPa. When doped with 2xE15cm-3 nitrogen, the material hardness and elastic modulus become 8.2 and 182 GPa, respectively. In a prior work[1] we found that N-CZ silicon wafers processed for denuded zone formation have three defect regions (I: near surface, II: similar to DZ, and III: bulk), where precipitate density and O and N concentrations profiles vary significantly. Both surface and cross-section indentations in grids of up to 50 indents were made using Berkovich indenter. Indentation grids made on the cross-section were distributed over the three regions. A combination of various loads and indenter tips were used in order to remove tip and load effects. One of the grids was done in the near surface with a Northstar indenter and smaller load. Correlation at the sub-micrometer level of the shallow oxynitride near surface layer local hardness with the O and N depth profiles was obtained. The measured elastic modulus and hardness of both N free and N doped samples significantly differ from

those of CZ Si. Indents made on the surface of annealed N-CZ wafer yielded similar average hardness and elastic modulus as those made on cross-section of Region I (near -surface). The former showed linear decrease of the hardness with the contact depth, in agreement with the latter. Region II (DZ) that has lowest O and N concentrations and Region III (indentation grid located at 150 μm depth) indented with the same load and the same tip have shown slightly harder bulk (12.3 GPa versus 11 GPa). The hardness correlates well with the measured O and N profiles. In addition, distinct high hardness values appeared in the data set and were attributed to precipitate hardening effects. Load controlled nano-scratch tests of N-CZ Si confirmed the existence of harder phases with a separation distance (0.8 μm). These include small precipitates, much smaller than 20 nm radius. The density of hard phase domains in N-CZ, estimated to 1E13 cm-3, matches the N related nuclei density recently found by a combination of Oxygen Precipitate Profiler and high resolution SIMS profiling.[2] [1] A.Karoui, F. S. Karoui, A. Kvit , G. A. Rozgonyi, Appl. Phys. Lett., 80(12), 2114 (2002). [2] A.Karoui, F. S. Karoui, G. A. Rozgonyi, D. Yang submitted to J. Appl. Phys.

P8.37

The role of shear in the onset of the bcc to hcp stress-induced martensitic transformation in Fe. Adrian Lew¹, Kyle Caspersen², Michael Ortiz³ and Emily Carter²; ¹Mechanical Engineering, Stanford, Stanford, California; ²Chemistry and Biochemistry, UCLA, Los Angeles, California; ³Aeronautics, Caltech, Pasadena, California.

Iron shows a pressure induced martensitic phase transition from ground state ferro-magnetic bcc to non-magnetic hcp at approximately 13GPa. The exact transition pressure is not known and is postulated to be strongly dependent on shear deformations. To understand the role of shear deformations on the transition onset we have developed a multi-scale Fe model that contains a quantum mechanics based free energy dependent upon all strain components, a kinematically compatible spinodal decomposition of phases, and a dependence on the bcc to hcp transition path(s). Using this model we see a strong dependence of the transition pressure with shear components of the deformation.

P8.38

Finite-Temperature Quasicontinuum Method: Application to Void Growth in Shocked Al. Jaime Marian, Jaroslav Knap and Michael Ortiz; California Institute of Technology, Pasadena, California.

Void growth and coalescence are known to be important ductile fracture mechanisms in metals. Under shock conditions, such as those encountered in explosively loaded materials, the attendant high deformation rates may induce the formation of spall layers characterized by a large concentration of nano and microvoids arranged in spatial patterns. The diffusion, growth and coalescence of these voids can lead to material failure under these extreme conditions. Therefore, a detailed understanding of the main mechanisms by which these voids grow and interact is required in order to construct reliable multiscale models of spallation in metals. The quasicontinuum (QC) method, due to its coarse-grained/atomistic capability to describe the material in terms of the deformation gradient, has proved a reliable means for obtaining the resulting dislocation structures and the equivalent constitutive relations in systems of realistic size containing large voids. However, to date, all calculations in QC are constrained energy minimizations and, thus, many of the thermally-activated phenomena associated with the plasticity emerging from the void is not captured by the method. Here, we apply coarsened Langevin dynamics within the latest QC formulation, both with fixed and variable timesteps. Preliminary results are presented for Al, and comparison with the static calculations is provided.

P8.39

A Three-Dimensional Multi-Phase Field Model of Dislocation Dynamics and Plasticity in Crystals. Pilar Ariza and Michael Ortiz; California Institute of Technology, Pasadena, California.

We present a model of discrete dislocation dynamics based on: a lattice-statics representation of crystal elasticity; and the introduction of eigen-deformations in order to represent the lattice-invariant or plastic deformations of a crystal. The formulation is fully three-dimensional and accounts for the complete complement of slip systems in bcc crystals, including (110) and (112) slip. We show that all plastic deformations can be represented in terms of a number of integer-valued phase fields, one per slip system, measuring the local slip activity. In particular, the value of a phase field at a point on a slip plane counts the number of dislocations in the corresponding slip system which have passed over the point. The present formulation may be regarded as a three-dimensional, multislip generalization of the phase-field theory of dislocation dynamics of Koslowski et al. (2002). However, the present theory differs in the important respect of

being based ab initio on a discrete lattice representation of the crystal. This renders dislocation core structures well-defined and obviates the need for postulating a Peierls potential. We show that, within the confines of the theory, discrete dynamics can be given a compelling interpretation in terms of discrete differential operators. Dislocation junctions and the degree of entanglement of the dislocation ensemble can also be understood in terms of homology groups and topological invariants, leading to a succinct formulation of forest hardening. A chief advantage of the theory is that it is analytically tractable. We take advantage of this feature to provide explicit solutions of deformation-induced sub-grain dislocation structures.

P8.40

Dislocation Nucleation at Heterogeneities of Crystal Surfaces. Guanshui Xu and Chengzhi Li; Department of Mechanical Engineering, UC Riverside, Riverside, California.

We will present an analysis of energetics of dislocation nucleation at heterogeneities of crystal surfaces based on the Peierls-Nabarro dislocation model. By modeling the surface heterogeneities as part of a three-dimensional crack surface, we transfer the half space problem into an equivalent three dimensional crack problem in the infinite space. The profiles of embryonic dislocations, corresponding to the relative displacements between the two adjacent atomic layers along the slip planes, are then rigorously solved through a previously developed variational boundary integral method. To quantitatively understand the effects of various surface heterogeneities such as cracks and steps on dislocation nucleation, we have determined the stress dependent activation energies required to activate dislocations from their stable to unstable saddle point configurations. A parametric study of step geometry on dislocation nucleation will be presented in detail. Compared to previous analyses of this type of problem based on continuum elastic dislocation theory, the presented analysis eliminates the uncertain core cutoff parameter by allowing for the existence of an extended dislocation core as the embryonic dislocation evolves. Because of the serious limitation of direct atomic simulation for this type of problem, the methodology of incorporating atomic information into continuum approach presented in this analysis appears to be particularly noteworthy for the study of the energetics of atomic processes involved in extended defects such dislocations and grain boundaries.

P8.41

Mesoscale Modeling of Plasticity of Irradiated Metals by Dislocation Dynamics. Masato Hiratani and Vasily V Bulatov; CMS/MSTD, Lawrence Livermore National Laboratory, Livermore, California.

Deformation behavior of irradiated metallic crystals is investigated by discrete dislocation dynamics. We developed physics based mobility laws for individual dislocation segments by implementing atomistic data such as temperature dependence of phonon drags or cross-slip energetics. Simulations are run for single crystals of size of 1 micron under either creep condition or constant strain rate condition for nickel, copper, and molybdenum samples. Low-intermediate dosage of irradiation is tested by placing the corresponding density of defect clusters (stacking fault tetrahedra, interstitial loops, perfect loops, etc.) within the simulation cell, together with low density of in-grown network dislocations. Results indicate dose dependence of mechanical responses such as hardenings and stress serrations. Moreover, complex patternings are revealed through signal processing of spatial distribution of dislocations or time series of strain, which are typical of open dissipative system. Role of thermal fluctuations and segment discretization during coarse graining will be also discussed. 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.

P8.42

Nanocrystalline Grain Growth due to Non-Linear Interface Kinetics. Moneesh Upmanu^{1,2}, Paul Martin³ and Anthony Rollett⁴;

¹Engineering Division, Colorado School of Mines, Golden, Colorado; ²Materials Science Program, Colorado School of Mines, Golden, Colorado; ³Mathematical and Computer Sciences, Colorado School of Mines, Golden, Colorado; ⁴Material Science and Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania.

Recent experimental studies have shown that thermal evolution of nanocrystalline interface microstructures is stable compared to parabolic grain growth observed in coarser microstructures. In this talk, we show that for initial stage growth of these microstructures, the driving force dependence of interface migration rates can no longer be assumed to be linear. We derive the modified growth law due to non-linear interface kinetics, and find that the linear growth observed in experiments is in excellent agreement with sublinear interface kinetics based grain growth predictions.

P8.43

Ultrasonically Assisted Nanoindentation for Thin Film Fatigue Characterization. Antanas Daugela, Oden Warren, Vytaitas Blechertas and Thomas J Wyrobek; Hysitron Inc., Minneapolis, Minnesota.

An ultrasonically induced nanofatigue phenomenon was employed to characterize multi-layered thin films. A quantitative nanoindentation device in combination with a specially designed ultrasonic transducer was used for characterization. Nanoindentation process was carried out on the sample attached to the standing-wave ultrasonic transducer oscillating at 200kHz. Ultrasonically induced film fracture due to fatigue was monitored on the quasi-static holding segment of loading-unloading curve as well as on in-situ Scanning Probe Microscopy (SPM) type images. A number of critical nanofatigue cycles was counted on the holding segment of quasi-static loading-unloading curve. A number of critical nanofatigue cycles required to delaminate coating can be a-priori calculated using Basquin's law modified for the elasto-plastic contact. The proposed method of ultrasonically induced nanofatigue phenomenon has a strong potential to characterize data storage thin films. Supporting experimental data and recommendations will be presented.

SESSION P9: Nanostructured metals and alloys-II

Chairs: Amiya Mukherjee and Yuntian Zhu

Friday Morning, April 16, 2004

Room 2004 (Moscone West)

8:15 AM P9.1

Ductility and Deformation Mechanisms of Nanostructured Al Alloys. Bing Q. Han¹, Farghalli A. Mohamed² and Enrique J.

Lavernia¹; ¹Chem Eng Mater Sci, Univ. of California, Davis, Davis, California; ²Chem Eng & Mater Sci, University of California, Irvine, Irvine, California.

Low tensile ductility is one of critical challenges facing the science and technology of nanostructured materials. As an example, despite the fact that high strength is frequently observed in bulk nanostructured aluminum alloys, ductility and work hardening are often observed to decrease with decreasing grain size. In the present study, the tensile ductility of bulk nanostructured aluminum alloys processed via several techniques is analyzed. Several approaches are proposed in an effort to improve ductility and the underlying physical mechanisms are discussed.

8:30 AM *P9.2

Plasticity and strength of nanocrystalline Ni and Ni-W alloys. T.G. Nieh¹ and Chris Schuh²; ¹Lawrence Livermore National Lab,

Livermore, California; ²Materials Science & Engineering, MIT, Cambridge, Massachusetts.

In this paper, both experiments and simulation results from nanocrystalline Ni with a grain size less than 20 nm are presented. The effect of grain size, the type of grain boundary, and alloying on the strength and plasticity will be discussed. Microstructure and impurity distribution in the nano-materials both before and after deformation are examined using techniques such as atom probe field ion microscopy (APFIM), electron energy loss spectroscopy (EELS) with a nano-probe, and high-resolution TEM with angular dark field (ADF) imaging capability (i.e. Z-contrast). Fracture mechanism in nanocrystalline materials will also be addressed. Tension-compression strength asymmetry in nanocrystalline metal will also be addressed.

9:00 AM P9.3

Direct Experimental Visualization of Grain Rotation Induced Grains Reorientation in PLD Nanocrystalline Ni. zhiwei shan¹,

James Knapp⁴, D. M. Follstaedt⁴, E. A. Stach³, M.K. Wiezorek² and Scott Mao¹; ¹Department of Mechanical Engineering, university of pittsburgh, pittsburgh, Pennsylvania; ²Material Science and Engineering, University of pittsburgh, Pittsburgh, Pennsylvania; ³LabNational Center for Electron Microscopy, Lawrence Berkeley, Berkeley, California; ⁴MS 1056, Sandia National Labs, Albuquerque, New Mexico.

Grain boundary-related deformation process is expected to exist at nanoscale grain sizes. In situ tensile tests in pulsed laser deposited Ni with an average grain (grain) size of about 18nm and a narrow grain size distribution was conducted in a 3010 transmission electron microscope. The investigation, for the first time, not only provided direct evidence confirming MD predictions of grain boundary related deformation processes but also revealed a unique deformation mechanism for nanocrystalline materials, i.e. grain rotation induced grains groups' reorientation. However, both the bright field observation during the deformation and the following high resolution electron microscopy exploration on fresh crack edge suggested that

the dislocation-based deformation still play its role for as deposited nanocrystalline Ni. The results underscore the cooperated deformation (deformation) mechanism for both grain boundary and dislocation activities and will have implications for interpreting the unusual mechanical behavior of the nanocrystalline materials.

9:15 AM P9.4

The Deformation Behavior of Fe-C Martensitic Steel Observed by in-situ Nanoindentation in a TEM.

Takahito Ohmura¹, Andrew M Minor², Eric A Stach² and John W Morris^{3,4}; ¹Steel Research Center, National Institute for Materials Science, Tsukuba, Ibaraki, Japan; ²National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, California; ³Department of Materials Science and Engineering, University of California, Berkeley, California; ⁴Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California.

The indentation-induced deformation behavior of Fe-C martensitic steel was observed through in-situ nanoindentation in a TEM in order to reveal the interaction of dislocations with grain boundaries. The sample was high-purity Fe-C binary martensite with carbon content of 0.4 wt%. The specimen was austenitized at 1323 K for 900 s and then ice-brine quenched followed by tempering at 723 K for 5400 s. The specimen surface was electrically polished and then thinned to electron transparency with a Focused-Ion Beam (FIB). The electrically-polished surface was coated with a Pt film before FIB milling in order to avoid damage to the surface from the incident Ga⁺ ions. The Pt film was then mechanically removed prior to indentation by breaking it off in situ with the nanoindenter inside the TEM. Indentations were made into the surface such that a specific low angle or high angle boundary would be visible beneath the indenter, and the deformation at that boundary could be observed. The low angle boundaries corresponded to martensitic lath boundaries, while the high angle boundaries presumably corresponded to packet boundaries or the boundaries between prior austenite grains. In the case of the low-angle grain boundary, dislocations were emitted near the indenter/specimen contact point, and then moved toward the grain boundary. Upon reaching the boundary, the dislocations piled up and could be seen to stop on account of the boundary. As the indenter penetrated further, a large number of dislocations were simultaneously emitted on the far side of the grain boundary into the adjacent grain. After withdrawing the indenter, a high density of dislocations remained near the grain boundary on the adjacent side of the grain. Dislocation interactions with the high angle boundary appeared to occur in a completely different manner as compared to the low-angle case. Once dislocations reached the high angle grain boundary, they disappeared at the grain boundary without any indication of specifically piling up. Furthermore, no dislocation emission occurred at the boundary in the adjacent grain side. The indented grain was heavily deformed while the adjacent grain showed little change in shape, which means that the indentation-induced deformation was limited to the indented grain and the deformation did not propagate easily from the indented grain to the adjacent grain. In summary, the high-angle grain boundary showed a high resistance to slip transfer, while the low angle boundary demonstrated easy slip transfer. These observations will be discussed in light of both the conventional and classical interpretations of grain boundary strengthening.

9:30 AM P9.5

The Role of Initial Microstructure in Large Strain Deformation of High Carbon and High Speed Steels.

Caroline C Swanson¹, Srinivasan Swaminathan¹, W Dale Compton¹, Srinivasan Chandrasekar¹ and Kevin P Trumble²; ¹School of Industrial Engineering, Center for Materials Processing and Tribology, West Lafayette, Indiana; ²School of Materials Engineering, Center for Materials Processing and Tribology, West Lafayette, Indiana.

Chip formation by machining provides a simple experimental configuration in which very large plastic strains can be imposed in a single stage of deformation and systematically varied, even in high strength metals and alloys. A study has been made of microstructure refinement in high carbon and high speed steels arising from the imposition of large plastic strains, with a particular focus on the effects of initial microstructure. Prior to machining, the initial microstructures of 1080 carbon steel and M2 high speed steel were varied by subjecting the steels to different heat treatments. Chips were then produced from these steels by machining. The deformation conditions were characterized by different levels of plastic strain, temperature and strain gradients in the deformation zone. Microstructure and hardness of the chip samples were assessed as a function of the initial microstructure and deformation parameters. It is found that under appropriate conditions of deformation, the resulting chip microstructure is nanocrystalline. The grain size, microstructure and hardness of the chips are related to the initial microstructure. The extent of grain size refinement observed in the chips indicates the potential of machining as a method for creating

ultra-fine grained steel microstructures.

9:45 AM P9.6

The Role of Vorticity in the Formation of Tribomaterial During Sliding. Karthikeyan Subramanian¹, Jian-Hui Wu¹, Xi-Yong Fu² and David A. Rigney¹; ¹The Ohio State University, Columbus, Ohio; ²Merck Research Laboratories, West Point, Pennsylvania.

The formation of tribomaterial during sliding is well documented for a wide range of materials. Transfer, adhesion, mechanical mixing and formation of nanocrystals are commonly reported, but the mechanisms involved have not been well understood. Recently, molecular dynamics (MD) simulations have been performed to obtain new information on the response of materials to sliding interactions. The results help to explain experimental observations on simple metals such as copper, bulk metallic glasses and multi-component nanocomposite coatings. When the sliding speed is sufficiently high, the strain rate allows vorticity to develop. It is suggested that the resulting eddies are largely responsible for frictional energy dissipation and mechanical mixing in both crystalline and amorphous materials and for the shear mixing of soft embedded particles in nanocomposite coatings. A comparison of eddy sizes with nanocrystal sizes in tribomaterial suggests that vorticity is directly responsible for the formation of such nanocrystal material. Similarities of flow behavior with that of fluids is noted.

10:30 AM *P9.7

Extraordinary Strength and Ductility in SPD-Produced Nanostructured Metals. Yuntain T. Zhu² and Ruslan Z. Valiev¹; ¹Institute of Physics of Advanced Materials, Ufa State Aviation Technical University, Ufa, Russian Federation; ²Los Alamos National Laboratory, Los Alamos, New Mexico.

Bulk nanostructured metals with a mean grain size of about 50-100 nm very often exhibit high hardness, but poor ductility. However, recent works demonstrate that extraordinary strength and ductility can be observed in nanostructured metals produced by severe plastic deformation (SPD). In this paper we show that the combination of high strength and ductility is originated not only from the presence of fine grains, but from the structure of grain boundaries and internal stresses. The origin and mechanisms of this phenomenon are studied in this work based on analysis of performed tensile tests and thorough microstructural studies. Special attention is focussed on studies of the defect structure of grain boundaries. This has allowed us to establish the features of highly non-equilibrium boundaries formed by means of SPD processing. Such non-equilibrium boundaries may lead to a change in mechanisms of nanomaterial deformation and development of grain boundary sliding at room temperature. This change in deformation mechanisms is responsible for exhibition of the observed unique mechanical behaviour of SPD metals.

11:00 AM P9.8

Grain Size Distribution Effect on Mechanical Behavior of Nanocrystalline Materials. Alla V Sergueeva, Nathan A Mara and Amiya K Mukherjee; Chemical Engineering&Materials Science Department, University of California, Davis, California.

Nanocrystalline materials generally exhibit increased strength in comparison to their coarser-grained counterparts, but at the expense of ductility. At low temperatures these materials with grain size below 50 nm fail in a brittle manner with near zero plasticity. High temperature deformation in the temperature range where the microstructure is stable results in a slight increase in ductility but is far from predicted superplastic behavior. Significant ductility of initially nanostructured materials is due to intensive grain growth whereupon the advantages derived from a nanostructured state disappear. These observations have been attributed to limited dislocation activity in the materials with nanocrystalline (less than 50 nm) grains indicated by an absence of work hardening, which in turn leads to mechanical instability. Ductility enhancements have been achieved in nanostructured metals through the incorporation of larger grains in a fine-grained matrix. These larger grains are responsible for strain accommodation and increased ductility while a fine-grained matrix provides the high strength of the materials. This investigation is supported by NSF, Division of Materials Research (grant NSF-DMR-0240144)

11:15 AM P9.9

Structure and Property Evolutions of ECAP processed 7075 Al alloy upon T651 and T7351 Treatments. Yonghao Zhao¹, Xiaozhou Liao¹, Yuntian Theodore Zhu¹ and R. Z. Valiev²; ¹Materials Science and Technology, Los Alamos National Lab., Los Alamos, New Mexico; ²Institute of Physics of Advanced Materials, Ufa State Aviation Technical University, Ufa, Russian Federation.

Evolutions of microstructure and mechanical tensile properties of

equal-channel angular pressing (ECAP) processed and coarse grained (CG) 7075 Al alloys upon T651 (annealed at 393 K for 48 h in Ar atmosphere) and T7351 (annealed at 486 K for 9 h in Ar after T651) treatments were investigated by x-ray diffraction (XRD), transmission electron microscopy (TEM) and tensile test. Upon T651 and T7351 treatments, the tensile stress of the ECAP processed sample decreased from 721 MPa to 604 MPa (T651) and 434 MPa (T7351), while for the CG sample, the tensile stress increased from 531 MPa to 592 MPa (T651) and then decreased to 530 MPa (T7351). XRD and TEM show that the enhanced tensile stress of the CG samples upon T651 treatment is mainly attributed to the second phase precipitation. For the ECAP processed samples, upon annealing the microstrain (dislocation density) decreased from 0.55 % to 0.2 % (T651) and 0.1 % (T7351), and the crystallites grew from 194 nm to 2000 nm (T651) and 4000 nm (T7351), which decrease the tensile stress, and overcompensate the precipitation strengthening. The obtained data indicate that in order to attain high strength by means of heat treatment of ECAP-processed Al alloys, standard regimes should be adjusted. New processing regimes leading to superior properties in ECAP-processed Al alloys are discussed as well.

11:30 AM P9.10

The Influence of the Misorientation of Grains and its Boundary Structure on the Strength and Ductility of Ultrafine-grained Cu: Model and Experiments.

Florian Hans Dalla Torre, Rimma Lapovok, James Sandlin, Elena V. Pereloma, Chris H.J. Davies and Peter F. Thomson; School of Physics and Materials Engineering, Monash University, Melbourne, Victoria, Australia.

The influence of the misorientation relationship of grains on the mechanical properties is investigated in ultrafine-grained copper processed by different routes of severe plastic deformation (SPD). After a certain number of passes by equal channel angular pressing (ECAP), the grain size remains constant. The degree of misorientation among grains increases, with narrowing boundaries, due to further deformation. It is suggested that high angle grain boundaries are favorable for increasing the tensile ductility in ultrafine-grained metals processed by SPD. This paper focuses on the influence of texture, grain misorientation and the change in the volume fraction of grain boundaries on the tensile properties of ECAP Cu. A reliable model incorporating the microstructural features has been developed to describe the mechanical properties. The change from non-equilibrium boundaries and cell walls into relaxed equilibrium grain boundaries is investigated by in-situ TEM annealing experiments. Tensile properties of annealed specimens having a relaxed microstructure are compared to the as-processed ones.

11:45 AM P9.11

Bimodal Structures and Deformation of Cryomilled Bulk Nanocrystalline Al-Mg Alloys using Experiments and Modeling.

Zonghoon Lee¹, Johnathan Lee¹, David Witkin², Enrique J Lavernia³ and Steven Nutt¹; ¹Department of Materials Science, University of Southern California, Los Angeles, California; ²Department of Chemical Engineering and Materials Science, University of California at Irvine, Irvine, California; ³Department of Chemical Engineering and Materials Science, University of California at Davis, Davis, California.

Cryomilled bulk nanocrystalline Al-Mg alloys with bimodal grain size were investigated using experiments and modeling. Bimodal Al-Mg alloys were prepared by blending of cryomilled nanocrystalline powder and unmilled coarse-grained Al-Mg powder, then consolidated by hot isostatic pressing and extrusion to produce bulk samples, resulting in high strength, enhanced ductility and toughness. The matrix was nanocrystalline, while the elongated coarse-grained bands were aligned along the extrusion direction. Samples exhibited increased ductility and toughness from the addition of a coarser-grained fraction while retaining high strength. FEM modeling of bimodal structures was performed to estimate the mechanical properties and to investigate the local deformation between nanocrystalline grains and coarse grains. The modeling results were comparable to experimental observations, providing a capability to design optimized bimodal structures. This process demonstrates a new approach to designing and producing bulk nanocrystalline metals that exhibit a combination of high strength and enhanced ductility and toughness. Designing bimodal (or multi-scale) structures with specific nano-scale phases, dimensions and morphologies will enable engineers to optimize select combinations of properties.