SYMPOSIUM BB
Material Instabilities and Patterning in Metals

April 17 – 18, 2001

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*Invited paper
8:30 AM *BB1.1
POLYCHROMATIC X-RAY MICROBEAM TECHNIQUES FOR
MICRON RESOLUTION 3-D STUDIES OF DEFORMATION IN
METALS. B.C. Larson, Solid State Div., Oak Ridge Natl Lab, Oak
Ridge, TN.

The ultra-high brilliance of 3rd generation synchrotron sources,
together with the development of high-resolution x-ray focusing optics,
amnimated with multi-keV x-ray microbeam software, and newly developed
depth-profiling techniques have made 3D x-ray structural microscopy
possible with micron resolution in all directions. Micron resolution
3-D x-ray structural microscopy (XSM) provides non-destructive
access to the atomic microstructure, shape, and stress/strain/texture of
metallic microstructure in both single and polycrystalline materials in
unstrained and deformed materials. The key elements of the technique
will be described and methods for obtaining micron depth resolution
will be discussed. Application of the technique to mesoscale
investigations of elastic and plastic deformation will be illustrated
through measurements on Si, Cu, and Al under deformed and
unstrained conditions as performed on the microbeam x-ray facility
developed on the MHATT-CAT beamline at the Advanced Photon
Source (APS). The complementarity of x-ray microbeam techniques to
electron microscopy and electron backscattering, and their relation
to computer simulation and multi-scale modeling of mesoscale
microstructure and evolution will be discussed.

Research sponsored by Oak Ridge National Laboratory, managed by
UT-Battelle, LLC, for the U.S. Department of Energy under contract
DE-AC05-00OR22725. MHATT-CAT is operated by the University of
Maryland, Lawrence Livermore National Laboratory, and
Lawrence Berkeley National Laboratory. The operation of the APS is
sponsored by the DOE.

9:00 AM BB1.2
DISLOCATON WALLS IN FINITE MEDIA: THE CASE OF AN
INFINITE SLAB. M.P. Sulehri and W.G. Wolfer, Lawrence Livermore
National Laboratory, Livermore, CA.

The dominant feature in dislocation patterns of deformed metals is a
cell structure of dislocation walls. Each wall is stabilized by
short-range interactions between dislocations. However, the
interaction forces which control the spacing of these dislocation walls
are still the subject of active research. Stable dislocation walls of
finite extent have stress fields which fall off exponentially over a
characteristic distance of h/2p, where h is the spacing between
dislocations within the wall, and is in general much smaller than the
cell size. As a result, various researchers have studied dislocation walls
of finite extent, but still embedded in an infinite elastic medium.

Finite dislocation walls do exhibit long-range stress fields which
decays over distances of order of the height of the wall. Dislocation walls in polycrystalline materials are naturally limited by the grain size.

Grain boundaries introduce strain incompatibilities which affect the
long-range stress field of dislocation walls. For example, grain
boundaries may project shear components of a dislocation stress
field. In order to study the importance of boundary conditions,
dislocation walls have been evaluated in ashl. We have treated two
sets of boundary conditions. In one set, shear stresses are reduced or
vanish on the slab surfaces, and in the second set both shear and
normal stresses are partially relaxed or vanish. In the former case,
dislocation walls will pass long-range shear stress fields with deep
troughs capable of capturing dislocations of opposite Burgers vector
and inducing the formation of a new dislocation wall. Relaxing normal
stresses also will reduce the strength of the troughs, but at the same
time produce a tilt angle that extends far from the wall.

9:15 AM BB1.3
USAXS IMAGING: A NEW X-RAY WINDOW ON DEFORMATION.
J. Levine, G.G. Long, R.J. Fields, NIST, Gaithersburg, MD.

New ultrasmall-angle X-ray scattering (USAXS) facilities at 3rd
generation synchrotron sources enjoy an additional 1 to 3 decades of
x-ray brilliance over 2nd generation sources, and can now quantify
microstructural features from 3 nm to 1.3 micrometers in size. These
developments offer exciting possibilities for further exploration of
dislocation and other deformation microstructures. A new
transmission X-ray imaging technique based upon USAXS is
described. The image is formed from X-rays that are scattered at
small angles by the density variations in the sample. USAXS typically
begins two to six decades below the intensity of the main
transmitted beam. The USAXS instrument selects X-rays from a
specified scattering angle (q value) and passes them to the imaging
channeling a quantum of information at different wavelengths within
the sample to be imaged. These data can then be correlated with quantitative

volume averaged results from a USAXS analysis. USAXS imaging is demonstrated on creep cavitites in polycrystalline Cu.

9:30 AM BB1.4
NANOLAMELLAR STRUCTURES IN A ROLLED Cu-Ag ALLOY.
M.T. Lytle and D.A. Hughes, Materials and Engineering Sciences
Center, Sandia National Laboratories, Livermore, CA.

The evolution of the microstructure and texture during deformation of
a directionally solidified Cu-Ag eutectic alloy is systematically
investigated. Both the copper and silver phases have the same initial
crystal orientation and an average dendrite spacing of 0.5 μm.
Following several rolling reductions, the microstructure and texture
are characterized. Large rolling reductions produce very small-scale
structures in both phases, shape, and stress/strain/texture of crystal
microstructure in both single and polycrystalline materials in
unstrained and deformed materials. The key elements of the technique
will be described and methods for obtaining micron depth resolution
will be discussed. Application of the technique to mesoscale
investigations of elastic and plastic deformation will be illustrated
through measurements on Si, Cu, and Al under deformed and
unstrained conditions as performed on the microbeam x-ray facility
developed on the MHATT-CAT beamline at the Advanced Photon
Source (APS). The complementarity of x-ray microbeam techniques to
electron microscopy and electron backscattering, and their relation
to computer simulation and multi-scale modeling of mesoscale
microstructure and evolution will be discussed.

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Maryland, Lawrence Livermore National Laboratory, and
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sponsored by the DOE.

9:45 AM BB1.5
LOCAL 3-D STRAIN AND ORIENTATION MEASUREMENTS IN
TENSILE STRAINED AND NANNONDENTED COPPER USING
X-RAY MICROBEAM MS. Weng Yang, B.C. Larson, G.E. Ice, J.Z.
Tischler, J.D. Budai, K.-S. Chang, Oak Ridge National Lab; D.A.
Hughes, Sandia National Lab; G.M. Pharr, University of Tennessee/ORNL; N. Tamura, Lawrence Berkeley National Lab;
W.L. Lew, Howard University.

We have used submonolayer resolution broad-band x-rays (white) x-ray microbeam and x-ray microdiffraction orientation
free x-ray microbeam X-ray microdiffraction to determine the local orientation and strain/flexure in deformed Cu samples within volume elements ~0.7 x 0.7 x 1.0 μm3.
Spatially-resolved x-ray microbeam Laue diffraction measurements made on 40 MPa tensile strained Cu single crystals have been
analyzed to determine lattice orientations and stress between dislocation walls in tensile strained Cu. The dislocation cell structure and
local lattice orientations observed using x-ray microbeam will be correlated with TEM observations, and stress levels associated with the plastic/elastic deformation and dislocation walls in the tensile strained copper will be discussed. The measurements on nanodented Cu were used to determine the spatial distribution of plastic deformation below the edge line and in the regions of Berkovich indenters. Combinations of several lattice rotation systems were
observed under the edge region, while nearly one-dimensional tilt were found below, and extending beyond, the flat faces of the
indenter. The experimental techniques for 3-D x-ray microscopy will be discussed and the potential of the method for fundamental
investigations of deformation will be considered.

Research sponsored by the Oak Ridge National Laboratory, managed by
UT-Battelle, LLC, for the U.S. Department of Energy under contract
DE-AC05-00OR22725; the operation of the APS is
sponsored by the DOE. WY, NF, and KSC were supported through the ORNL
postdoctoral Research Program administered jointly by Oak Ridge
National Laboratory and Oak Ridge Institute for Science and
Education.

10:30 AM *BB1.6
IN-SITU NUCLEAR MAGNETIC RESONANCE AND TEM
INVESTIGATIONS OF MOVING DISLOCATIONS.
Jeff Th. de Hessen, Department of Applied Physics, Materials Science
Center and Netherlands Institute of Metals Research, Nijmegen,
THE NETHERLANDS; Omar Knecht Institute of Physics, University of
Dortmund, Dortmund, GERMANY.

The present paper reports new results on the dislocation dynamics
measured using a complementary new technique for metals and
In-situ nuclear magnetic resonance (NMR), that was
introduced by us in the past. The method is essentially based on the
interaction between nuclear electric quadrupole moments and
Other experiments support these ideas. The experiments, however, are
usually performed on materials cold-worked at various temperatures.

The paper will show that in-situ nuclear magnetic resonance is an excellent experimental method to study the actual kinetics involved. In this
investigation we focus on plastic deformation experiments at straining
For many crystal orientations, deformation induced extended planar dislocation boundaries separated by a few micrometers lie on planes approximately parallel to the slip planes. They are however not exactly aligned. The aim of the present study is to correlate the deviations of the boundaries from the slip plane with the active slip systems. The deviation is characterized in terms of the axis around which the boundary planes are rotated away from the slip plane and the direction of this rotation for the respective slip systems in each band. The focus of the work is on the geometric relation between slip systems and the deviation. In particular the occurrence of low-angle boundaries has previously been found in tensile deformed copper single crystal of other orientations and in tensile deformed polycrystalline aluminum but the results for these materials conflict.

11:30 AM BB1.9
AVALANCHE DYNAMICS IN COLLECTIVE DISLOCATION MOTION: EXPERIMENTAL EVIDENCES
Jerome Weiss, LGGE, CNRS, St Martin d’Heres, FRANCE.

A statistical analysis of the acoustic emissions induced by dislocation motion during viscousplastic deformation of ice is presented. The recorded acoustic emissions provide an accurate picture of the dynamic energy dissipated during dislocation motion. Creep as well as controlled strain-rate experiments indicate that collective dislocation dynamics during viscousplastic deformation is a complex, intermittent and inhomogeneous process characterized by avalanches in the motion of dislocations. These dislocation avalanches are controlled by the internal stresses and dislocations acting as stress sinks. The resulting dislocation structures are analyzed with transmission electron microscopy.
typical size of the cells increases as annealing takes place (the smaller cells shrink and disappear from the structure). In the spirit of a bottom-up and condition-dependent approach, a new simulation methodology is suggested, in which the discrete moving objects are dislocation wall segments rather than individual dislocations. The most important role governing the dynamics of the dislocation walls is local conservation of the net Burger's vector. The new coarse-grained simulation method is designed to give much closer correspondence with the 'microscopic' discrete dislocation dynamics results than previously available approaches.

2:15 PM *BB2.3* CRITICAL BEHAVIOR OF A STRAIN PERCOLATION MODEL IN METALS Y. Shiue1, N. E. Levine2, R. Thomas2. 1Center for Simulation of Materials, University of Pennsylvania, Philadelphia, PA 2Materials Science and Engineering, California Institute of Technology, Pasadena, CA

Using a single strain percolation model for a deforming metal, we show that the total strain exhibits critical power-law behavior near the critical point, which is well explained by the 2D strain percolation theory. The universal behavior results from 1) the large geometrical correlation length compared to the small strain correlation length and 2) attempt of the system to selforganize around the minimum stable strain. We also find a deviation from the universality class such that, as the initial strain increases, the probability distribution for the total strain changes from a power-law decay to an asymptotic bell-shape function. Other critical aspects of the model are also discussed.

2:30 PM *BB2.4* A PHASE-FIELD THEORY OF DISLOCATING DYNAMICS, STRAIN HARDENING AND HYSTERESIS IN DUCTILE SINGLE CRYSTALS. A.M. Cuitiño, Rutgers University, Dept of Mechanical and Aerospace Engineering, Piscataway, NJ; M. Koslowski, M. Ortiz, California Institute of Technology, Graduate Aeronautical Laboratories, Pasadena, CA; L. Stainier, University of Liège, Laboratoire de Techniques Aéronautiques et Spatial, Liège, BELGIUM.

A phase-field theory of dislocation dynamics, strain hardening and hysteresis in ductile single crystals is presented. Specifically, we consider the formation of large numbers of dislocations within a discrete slip planes through random arrays of point obstacles under the action of an applied shear stress. The theory rests on a variational framework for dissipative systems and accounts for energetic and kinetic effects. The energetics of the system is approximated by recourse to a screening assumption. The kinetics of the system stem from the assumed frictional interaction between dislocations and point obstacles. The phase-field representation enables the tracking of complex geometrical and topological transitions in the dislocation ensemble, including dislocation loop nucleation, bowing-out, pinning, and the formation of Orowan loops. The theory predicts a range of behaviors which are in qualitative agreement with observations, including: hardening and dislocation multiplication in single slip under monotonic loading; Taylor scaling, both under monotonic loading and, in an appropriate rate form, under cyclic loading; the Bauchinger effect under reverse loading; the fading memory effect, whereby recovered dislocations gradually relax via the influence of previous loading; the evolution of the dislocation density under cycling loading, leading to characteristic 'butterfly' curves; and others. The theory permits the coupling between slip systems; the consideration of obstacles of varying strengths; and dislocation line-energy anisotropy.

2:45 PM *BB2.5* GRAIN BOUNDARY SLIDING, MIGRATION AND DISLOCATION ACTIVITY IN NANOCRYSTALLINE METALS DURING DEFORMATION: A MOLECULAR DYNAMICS INVESTIGATION. Helena Van Swygenhoven, Peter Derlet, Paul Scherrer Institute, SWITZERLAND; Alfredo Caro, Centro Atómico Bariloche, ARGENTINA.

Large scale molecular dynamics computer simulations of 3-D nanocrystalline Ni and Cu metals with mean grain sizes ranging from 3 to 20 nm are performed. An analysis of the structure and energetics of the grain boundaries and triple junctions is presented using direct visualization, energy calculations and local crystallographic analyses. Grain boundaries are essentially similar to those found at the macro-scale, i.e. similar structural units are found, providing evidence against the view of grain boundaries in nano-crystals as liquid-like interfaces. Modeled samples are deformed by constant uniaxial tensile stress. A change in deformation mechanism is observed: at the smallest grain sizes all deformation modes are accommodated at grain boundaries, and grain boundary sliding resulting from the combined action of individual atomic jump processes, takes place. At larger grain sizes (above 12 nm), a combination of grain boundary sliding, migration and intragranular deformation activity is observed in this regime to address the microscopic view of sliding. When a homogeneous shear stress is applied across the interface between two grains, local stresses make each atom feel a different value of the net force acting on them, so that the resulting evolution of the equilibrium configuration, contributing in this way to a very small amount of the total plastic strain. Other observed mechanisms responsible for the plastic deformation, such as grain boundary migration and partial dislocations. The new understanding of dislocation dynamics and their relative importance as function of grain size and grain misorientation is determined.

3:30 PM *BB2.6* DISLOCATION, GRADIENTS, AND SIZE EFFECTS. Elias C. Altshuler, Laboratory of Mechanics and Materials, Polytechnic School, Aristotle University of Thessaloniki, GREECE; Center for Mechanics and Materials, Michigan Technological University, Houghton, MI

The role of inhomogeneous evolution of dislocation densities on the development of strain gradients in constitutive equation of plasticity is discussed. An interpretation of size effects is given on that basis.

4:00 PM *BB2.7* A MICROSCOPIC THEORY OF SUBGRAIN DISLOCATION STRUCTURES, MICROSTRUCTURAL SIZE, EFFECTIVE BEHAVIOR AND GRAIN-SIZE EFFECT. Sylvie Aubry, Michael Ortiz, California Institute of Technology Pasadena, CA.

We develop a micromechanical theory of dislocation structures and finite deformation single crystal plasticity based on the direct determination of dislocation microstructures and the computation of the attendant effective behavior. Specifically, we aim at describing the lamellar dislocation structures which develop at large strains under monotonic loading and the labyrinth, mosaic, fence and carpet structures which develop in fcc metals fatigued in double slip. These microstructures are regarded as instances of sequential lamination and treated accordingly. The present approach is based on the explicit construction of microstructures by recursive lamination and their subsequent equilibration in order to relax the incremental constitutive description of the material. The microstructures are permitted to evolve in complexity and fineness with increasing microscopic deformation. The dislocation structures are deduced from the plastic deformation gradient field by recourse to Kroner's formulas for the dislocation density tensor. The theory is rendered nondocal by the consideration of the selfenergy of the dislocations. Selected examples demonstrate the ability of the theory to: predict the full set of slip laws which are observed in fatigued specimens; predict the experimentally observed misorientation distribution functions; determine the effective behavior of crystals with microstructure; determine the size of the microstructures as a function of strain; and predict scaling relations such as the Hall-Petch effect.

4:15 PM *BB2.8* ASPECTS OF GRAIN SIZE STRENGTHENING IN POLYCRYSTALS. Dilig Chandrasekaran, Kjell Pettersson, Dept of MSE, Royal Institute of Technology, Stockholm, SWEDEN.

The strengthening effect of grain boundaries is well established and observations of Hall-Petch effect and the microstructural mechanisms for the phenomenon are reviewed critically. A number of different models, relating the yield and flow stress in tension to various microstructural parameters in polycrystals, are reviewed and their predictive capabilities are evaluated. The focus is towards deformation at small strains and specifically the onset of plastic deformation, with special attention devoted to the specific role of grain boundaries. The fundamental implications of the different approaches are discussed with reference to two different classes of materials: 1) Materials with locked dislocations (e.g. steels) 2) Materials without locked dislocations (e.g. copper and aluminium).

Theoretical implications of the different approaches are compared with experimental results and conclusions are drawn concerning the applicability of the different models.

4:30 PM *BB2.9* NONLOCAL MODELS OF LOCALIZED PLASTIC FLOW DISCRETE DISLOCATION VS CONTINUUM DESCRIPTIONS. E. van der Giessen, Delft Univ of Technology, Delft, NETHERLANDS; A. Needleman, Brown Univ, Div Engineering, Providence, RI

Standard continuum descriptions of localized plastic deformation, e.g. in coarse slip bands at small strains or large strain shear bands, suffer from the absence of a material length scale. Gradient-type nonlocal models have attracted much attention in recent years, but their range of validity remains to be established. Discrete dislocation models are inherently nonlocal as they incorporate several physical length scales, and therefore hold the promise of rationalizing flow processes such as the spacing and thickness of slip or shear bands. Focusing
attention to small strains and two-dimensional problems, we discuss a
discrete dislocation methodology that allows for the solution of the
relevant boundary value problems. Several examples will be discussed
to illustrate the development of plastic deformation in localized
bands, such as during bending of a single crystal, and we analyze their
spreading. Also we present results of simulations where interfaces
provide barriers to slip. The associated dislocation boundary layers
and their evolution on a length scale and we investigate to what extent these can be described by
gradient-type continuum theories.

SESSION B33 POSTER SESSION
DEFORMATION AND PATTERNING AT SMALL SCALE: MODELS AND EXPERIMENTS
Chair: Hassin M. Zib
Tuesday Evening, April 17, 2001
8:00 PM
Salon 1-7 (Missouri)

B33.1
MACROSCOPIC SHEAR BANDING IN AN ALUMINUM-BASED ALLOY DURING EQUAL-CHANNEL ANGULAR PRESSING
Jinghao Wang, Xinhong Xu, Linkang Wang* and Haibo Wang, School of Metalurgy Xi’an University of Architecture & Technology, PR
CHINA. *Now at School of Mechanical Engineering, Xian Jiaotong University, PR CHINA.

Equal-channel angular pressing is now recognized as an effective
technique for fabricating materials with unique structures. It is
considerably less expensive compared to other manufacturing
techniques. However, the deformation behavior is strongly affected by different ECA
pressing routes. This paper presents the influence of the ECA
pressing routes on the microstructure and properties ofAl-5Si-4Cu alloy.

B33.2
INSTABILITY OF BUCKLING PATTERNS: FROM STRAIGHT-SIDED TO WORMLIKE STRUCTURES
F. Clermont, J. Colin, C. Guisset, J. Grillo Paters University, Futurescope, FRANCE.

The stability of buckling patterns of stainless steel thin films
deposited on polycarbonate substrates has been investigated by
atomic force microscopy. The specimens were deformed under uniaxial
compression of the substrate to generate straight-sided wrinkles
perpendicular to the applied stress axis. On release of the external
pressures, the wrinkles evolve at room temperature and pressure from
straight-sided to wormlike structures. Moreover this secondary
buckling in the perpendicular direction occurs with a significant
increase in width. A model based on energy calculation in the frame
of thin plate theory is proposed to determine analytically critical
stress values favourable to the wringing of straight-sided blisters.

B33.3
A GENERALIZED MODEL OF THE YIELD DROP IN IMPURE SEMICONDUCTORS: Boris Potekhin, Institute of Crystallography,
Russian Academy of Sciences, Moscow, RUSSIA.

The yield drop in semiconductors is the most pronounced transient
deformation instability. However, for silicon, the classic
Alexandrov-Hansen model of the walehke dislocation multiplication,
qualitatively good, does not describe some features of the
phenomenon, for example, the obvious difference in behavior of
Cruchysh simulation, which is marked by an increase in the 

crystaline material but also of novel class of materials - bulk metallic
glasses. Mechanisms of deformation and failure have been studied on
the yield drop of bulk amorphous metal. Figure 1 shows an example of the
3 mm diameter and 9 mm height were strained in the uniaxial
compression with a strain rate of 0.163 mm/min at temperatures 300,
77, and 4.2 K. At 300 K the plastic deformation has a neck-like
character. Plastic deformation is realized by localized glide bands.

B33.4
DEFORMATION INSTABILITIES IN BULK AMORPHOUS ALLOYS. Elena Tabachnikova Institute for Low Temperature Physics &
Engineering, Kharkov, UKRAINE; Maria Mcнал, Hans-Meiser Institutt, Berlin, GERMANY; Josef Minich, Kornel Cich, Institute of
Experimental Physics, Kosice, SLOVAKIA.

Unstable character of plastic deformation is typical not only of
crystaline material but also of novel class of materials - bulk metallic
glasses. Mechanisms of deformation and failure have been studied on
the yield drop of bulk amorphous metal. Figure 1 shows an example of the
3 mm diameter and 9 mm height were strained in the uniaxial
compression with a strain rate of 0.163 mm/min at temperatures 300,
77, and 4.2 K. At 300 K the plastic deformation has a neck-like
character. Plastic deformation is realized by localized glide bands.

B33.5
THE INTERACTION OF A CIRCULAR DISLOCATION PILE-UP WITH A SHORT RIGID FIBER: A 3-D DISLOCATION DYNAMICS
SIMULATION. Tarig A. Khrashi, Department of Mechanical
Engineering, University of New Mexico, Albuquerque, NM; Hassin
M. Zibib, School of Mechanical and Materiak Engineering,
Washington State University, Pullman, WA.

Three-dimensional simulations of the interaction of a circular
dislocation pile-up with a short rigid fiber have been performed. The
simulations represent an extension to the capabilities of a recently
developed discrete dislocation dynamics code. Such an interaction
may be of importance in metal-matrix composites, for example. Here
we consider an immersed short rigid fiber in a softer matrix, as well as
applied stresses, the equilibrium configuration of an initially un-equilibrated
circular dislocation pile-up around the fiber is captured dynamically.

B33.6
STABILITY OF DISLOCATION SUBSTRUCTURES AT DEFORMATION TEMPERATURE VARIATION AND
MECHANICAL PROPERTIES OF TITANIUM IN RANGE 4.2-373 K. Y. Y. Mosklenko, A.R. Smirnov, V.N. Kovalyov, B.I. Pogorelov,
Low Temp. Phys. & Eng. NAS of Ukraine, Kharkiv, UKRAINE.

The behavior of strain hardening curve reflects a plastic deformation
process as an evolution of nucleating and intersecting dislocations. If
the value of yield strength is conditioned mainly by chemical
composition and structural state of material then strain hardening
effect along stress-strain curve and true rupture stress is caused by
the yield drop of deformation-induced substructures. Substructure
state is an important factor also. In this work correlation between
predeformation-induced substructure and mechanical properties
of titanium with changing deformation temperature in range 4.2-373 K
have been studied. It has been established by electron-microscopy
that two main types of deformation-induced substructures form in
aluminium. One of them [ at low temperatures below 160 K]

present chaotic-distributed straight segments of screw dislocations,
they play role of background for a rising twin layers at deformation
strength >25%. During further deformation process of twinning strongly
activizes and provides up to 50% of whole low-temperature plasticity
of titanium in fact. Such structural state provides sufficient increasing
of yield strength and true rupturing stress as compared to the
unofected material.
substructure. Consisting of quasi-periodic walls of edge dislocations of the opposite sign orientation bands are unstable during subsequent deformation into temperatures [below 1000 °C] that is high mobility of edge dislocations. Therefore, predeformation-induced substructure of the type has not sufficient hardening influence on mechanical properties of titanium at low temperatures.

**DB3.7**

**DUCTILE CATASTROPHIC SHEAR FAILURE THROUGH ADEHABILITATING SHEAR BANDING IN ULCOSTRUCTURED TITANIUM**

**MANUFACTURED BY SEVERE PLASTIC DEFORMATION**

Vladimir Bengis, Institute for Low Temperature Physics & Engineering, Kharkov, UKRAINE; Josef Maksiı, Kornel Onch, Institute of Experimental Physics, Kosice, SLOVAKIA; Vladimir Stolyarov, Rushan Valuev, USATU, Ufa, RUSSIA

Nanostructured Ti with a 100 nm average grain size was manufactured by the equal channel angular pressing of the commercially pure titanium (CP-Ti) (with 15 mc% average grain size) followed by the thermomechanical treatment. Being strained by uniaxial compression at 300, 77 and 4.2 K it demonstrated yield stresses two times larger than CP-Ti and a little smaller ultimate plasticity (up to 30% to 77 K). Phenomenon of the ductile catastrophic shear failure was observed at all studied temperatures at the failure compressive stresses ranging from 1.4 to 2.4 GPa. Shear failure surfaces were oriented nearly at 45° to the compression axis. SEM fractography revealed a “vein pattern” at all observed shear failure surfaces. Such “vein pattern” is known in fractography of metallic glasses. It is a result of multiple necking during rupture of the hot superplastic material in the local catastrophic shear band. In metallic glasses “vein pattern” formation follows extreme local adiabatic heating of the bulk of the catastrophic shear band, caused by the high value of the failure stress and near sound velocity of catastrophic shear. In our case observed “vein pattern” formation could be indicated as indirect indication of extreme local heating during ductile shear failure of nanostructured Ti. Probably similar phenomenon was observed by H.G. Wildsoe and D.D. Mikhail in polycrystalline alloy Ti64/6V/4Al under tension (Acta Met., 1987, v 21, p. 1299). Our observations of non-uniform space distribution of “veins” on the shear failure surface of nanostructured Ti found dependent on the structure of failed samples. This non-uniformity considered followed from non-uniform local heating and the catastrophic shear band. Similarity of observed phenomenon to the ductile shear failure of metallic glasses allows to suppose that this micro mechanism of a ductile shear failure in nanostructured Ti is similar to that in metallic glasses and consists in avalanche shear spreading by grain boundary dislocations in nanostructured Ti.

**DB3.8**

**STRESS PATTERNS OF DEFORMATION INDUCED PLANAR DISLOCATION BOUNDARIES**

Shafique M.A. Khan, Hussein M. Zbib, School of Mechanical and Materials Engineering, Washington State University, Pullman, WA; Darcy A. Hughes, Center for Materials and Engineering Sciences, Sandia National Laboratories, Livermore, CA

Different types of dislocation structures are produced during deformation of metals, that are important in terms of their effect on the mechanical properties such as strain hardening and anisotropy. One of these deformation dislocations structures is nearly planar dislocation boundaries that separate regions of different slip thereby accommodating the stress field of the active slips. Such dislocation boundaries are known as geometrically necessary boundaries (GNBs). The internal structure (Burgers vector and line sense) of GNBs is characterized by boundary misorientation axes and boundary normal, which can be deduced from transmission electron microscopy (TEM) using Kikuchi analysis pattern. In the present study, misorientation axis and boundary normal are determined from TEM, and this experimental data is used in input to Frank’s formula, giving the stress contours that make up the boundary. The self-stress patterns for such infinite boundaries with general Burgers vector and line sense are constructed using the standard cases such as pure tilt boundary. The self-stress field of such finite boundaries is also investigated using dislocation dynamics simulations with emphasis on how finite size in real boundaries affects the stress pattern.

**DB3.9**

**THE CALCULATION OF ENERGETICAL PROFILE OF THE SHEAR IN THE ALLOYS WITH THE SUPERSTRUCTURE D019**

Michail A. Borisov, Veronica V. Rumyanchenko, Evgeniya V. Chernykh, Michail D. Strocastovich, General Physics Dept. Khar'kiv State Technical Univ.

The calculation of energetical profile of the shear in the alloys with the superstructure D019, based on the hexagonal closed packed lattice, is made by the method of computer simulation on the example of the alloys Mg12Ca and Ti5Al. The interaction between atoms in the alloys is given by the sets of pair semiparametric interatomic potentials, besides the connections of A-B type are described by the potential, taking into account the misfit of crystal lattice of hcp. At the orientation of shear in bicrystals in the directions <210>, <10 – 10>, and <10 – 12> the potential profiles appear to be different. Two quasi periods, corresponding to the shear of semibicrystals from 0 to all/2<210>, and from 0 to all/2<10 – 12>, were all is the parameter of alloy crystal, are found at the energetical profile. According the results of computer experiment possible dislocation reactions, taking place in the alloys, are given in this paper. The problems of dislocation interaction and strengthening of similar alloys are determined by the found dislocation reactions. The calculated values of the energy of planar defects, accompanying the dislocation reactions, are presented in the present paper.

**DB3.10**

**MICROMECHANICS OF PLASTIC FLOW LOCALIZATION AND FRACTURE IN SOLIDS**

Valery P. Kiel, Inst of Solid State Physics, Chernogolovka, Moscow District, RUSSIA

It is shown that the relationship between the stresses to start the motion and multiplication of dislocations of the same as for the stresses to initiate the first microcrack and microcrack, respectively, under different tests. It should be noted that this scaling is strictly fulfilled for data published on alkali halides, diamond-like carbon, semiconductors and metals, ceramics, etc. It is shown that cross-slip and climb mechanisms govern the localization of plasticity and the subsequent properties of fracture mode and structure of fracture surfaces in solids. This scaling indicates the controlling role of the deformation stress and the universality of dislocation cross-slip and climb mechanisms in the structure of metallic glasses and other materials. The characteristics of cross-slip and climb processes correlate with proper structures of fracture surfaces and explain the brittleness to ductile transition. In some cases the precursor deformation effects (due to generation of matrix defects before fracture may be considerable that they can noticeably change the character of temperature, grain-size, impurity content dependences of fracture parameters in comparison with the parameters of plastic flow like it was observed at different levels of the flow stress in the stressed materials.

**DB3.11**

**MODES OF PLASTIC DEFORMATION AND MICROSTRUCTURAL EVOLUTION**

Valery P. Kiel, Inst. of Solid State Physics, Chernogolovka, Moscow District, RUSSIA

The damping character of dislocation (D) unpinning, motion and multiplication irrespective of testing parameters exhibits the ultimate mean paths (UMP) of dislocations determined by test and sample history. Then dislocations exposed to multiplication thus forming the slip lines, bands, walls and subgrains, low-angle grain boundaries, interfaces (LAGB) due to cross-slip and climb of D. The rise of stress results in the decrease of cell sizes/D-spacing in slip bands, walls, LAGB, etc., thus transforming the LAGB into high-angle grain boundaries (HAGB) up to twinned, nanocrystalline, then mesostructured, fractures and damage. The scaling behavior of the reciprocal dependences of grain sizes, spacings of twins and SB, mean dislocation paths and their spacings in SB, walls, grain interior and LAGB, nanostructures of heavily deformed up to fracture versus the applied stress comply with universality of dislocation mechanisms of all deformation modes at atomic/meso- and macroscopic scale lengths for various crystal classes, processing and tests. Next finding of this work is the scaling between the deformation stresses of various stages of plasticity and fracture (at atomic, meso- and macroscopic scales) and the close correlation between the fracture surface roughness and deformation properties in alkali halide poly- and single crystals, severe deformed alloys (nanocrystals) and amorphous solids, ceramics under different tests/environments. This universal correlation is fulfilled in the widest range of temperature, stress and stress rate ranges (up to the shock wave stresses), for crystalline and disordered materials, etc.

**SESSION BB4: DEFORMATION PATTERNING AND LOCALIZATION**

Chairs: Geoffrey H. Campbell and Maximo Victoria

**Wednesday Morning, April 18, 2001**

**Golden耤reconomics (Main Hall)**

**8:30 AM**

**BB4.1**

**ROLE OF MICROSTRUCTURE IN PLASTIC FLOW LOCALIZATION**


The phenomenon of plastic flow localization has been observed in many metals and alloys in the unirradiated as well as irradiated...
conditions. In cases dominated by this mode of deformation, materials may exhibit sudden yield drop followed by negative work hardening and may suffer plastic instability and loss of ductility.

Commonly, this mode of deformation is found to be prevalent at temperatures below the recovery stage V. Such deformation behaviour is often attributed to the neutron irradiated materials and has been a matter of serious concern regarding their application in structural components of fusion and fission reactors. In spite of the fact that over the years a considerable amount of effort has been spent on studying the mechanical properties of irradiated materials, the understanding of physical mechanisms involved in the irradiation-induced defect clusters (or microstructure) and the flow localization has remained unclear.

The aim of the present review is to clarify the origin and ensuing consequences of the flow localization, first of all of a critical review of the relevant experimental observations will be presented. These observations will be analyzed in terms of the available theoretical models and the results of computer simulations of interaction between dislocations and irradiation induced defect clusters/loops.

9:00 AM BB4.2
RADIATION HARDENING AND PLASTIC INSTABILITY IN NEUTRON IRRADIATED METALS AND ALLOYS. Dan Edwards, Pacific Northwest National Laboratory, Richland, WA, Bishu Singh, Risø National Laboratory, Materials Research Department, Roskilde, DENMARK.

Irradiation hardening in metals and alloys is an important phenomenon that has been studied for over 40 years, but only recently have there been significant efforts to apply our knowledge of cascade damage to understanding the effect of irradiation on microstructure and hardening. In the context of this paper we will limit ourselves to the temperature regime (T < Stage V) where hardening is due to the presence of finite, non-size defect clusters. Under such conditions, the SIA (self-interstitial atoms) are segregated on the periphery of the core, leaving the core of the cascade vacancy-rich. This spatial inhomogeneity produces both sessile and sessile SIA clusters. The presence of highly mobile glissile clusters has profound consequences upon the microstructural evolution and the subsequent effect on hardening. Recent studies have shown that the SIA clusters can segregate in the form ofrafts ofdislocation loops, patterned arrays ofdefects, and more importantly from the standpoint of hardening, they can decouple grown in dislocations.

In most irradiated metals and alloys there is a threshold dose at which a yield drop becomes visible, which may be followed by a yield plateau and varying degrees of work hardening depending on the dose, irradiation and test temperature. Beyond this dose, the ability of the material to deform homogeneously also begins to disappear, leading to a tensile instability that involves localized deformation in channels or slip bands. The increase in strength also tends to saturate above a critical dose, but this dose may be different than the threshold dose for yield drop formation. In this paper we will present tensile data illustrating the tensile behavior of irradiated pure copper, precipitation hardened Cu-40 and Al-316 stainless steel as a function of neutron dose. This tensile behavior will be discussed within the framework of the two current models available to us, one of which relates the hardening to the accumulated clusters in the matrix acting as Orowan killers and more importantly from the standpoint of hardening, they can decouple grown in dislocations (Dispersed Barrier Hardening), and the other considers the possibility of the pinning of dislocation sources (Cascades-Induced Source Hardening).

9:15 AM BB4.3
ATOMIC INTERSTICIAL INFLUENCE IN PLASTIC FLOW LOCALIZATION IN IRRADIATED METALS. Brian D. Werth and Tomas Diaz de la Rubia, Lawrence Livermore National Laboratory, Livermore, CA.

Flow localization in metals is attributed to the annihilation of defect cluster obstacles by gliding dislocations and leads to highly localized deformation in narrow, obstacle free channels. The channels experience higher hardnesses, but overall specimen failure occurs at low uniform ductility and total strain. Plausible explanations for flow localization in irradiated fine centered cubic metals involve the absorption of individual vacancies from stacking fault tetrahedra by gliding dislocations and dislocation cross-slip. However, a conclusive atomic picture is lacking. In this work, we present the results of molecular dynamics simulations of the interaction of stacking fault tetrahedra with self-interstitial clusters as well as perfect and jiggled dislocations. The simulations are performed using embedded atom method interatomic potentials and provide atomic insight into the mechanisms responsible for flow localization in irradiated metals. This work is performed under the auspices of the U.S. Department of Energy and Lawrence Livermore National Laboratory under contract No. W-7405Eng-48.

9:30 AM BB4.4
DEFORMATION MICROSTRUCTURE EVOLUTION IN SINGLE CRYSTAL ALUMINUM. Michael F. Swage, Donald E. Kramer, and E. Levine, National Institute of Standards and Technology, Gaithersburg, MD.

Localized deformation and the formation of complex dislocation structures play a significant role in the room temperature flow behavior of high stacking fault energy FCC metals. Previous studies on the evolution of dislocation microstructures in Al have focused primarily on coiled polycrystalline material. In this study, the slip line evolution and underlying dislocation microstructures of high purity single crystal Al have been investigated. Atomic force microscopy investigations of surface slip bands were performed during deformation of Al single crystals with an evolved dislocation structure. These results have been compared with the deformation microstructures observed in thin films ex situ, by Transmission Electron Microscopy. Relationships between the observed surface structures and the presence of Geometrically Necessary Boundaries (GNBs) and Indentation Dislocation Boundaries (IDBs) will be discussed. Effects of crystallographic orientation on the slip line evolution and the nature of these dislocation structures will also be presented. The impact of these results will be discussed with respect to an ongoing modeling effort of plasticity in dislocation cell-forming FCC metals.

9:45 AM BB4.5
DEFORMATION BAND VELOCITIES AND LOCAL STRAIN RATES IN A Ni-Co-Fe ALLOY (INCONEL). Harry N. Jones, C.R. Pem, Naval Research Laboratory, Materials Science and Technology Division, Washington, D.C.

Nickel base alloys with nominal compositions similar to 70Ni-30Cr-15Fe, commonly referred to as INconel, exhibit serrated flow (Portevin-LeChatelier effect) in the temperature interval of 680-700°C. Within this temperature range a complex series of thermally activated processes can also be observed when a wire specimen of the alloy is heated with a controlled dead weight loading. These effects include the expected initial period of plastic deformation at the start of heating followed by its complete arrest at a higher temperature, a behavior that is completely out of sync with models for the thermal activation of plastic flow in metals. As the temperature is increased after this initial arrest a cascade of two or three large plastic instabilities involving high velocity propagation of narrow deformation bands is observed. Measurements of the band velocity using the time of flight within a 50.8 mm gauge length extensometer indicate that the velocity approaches 2.5 m/s in some cases. Estimates of the localized strain rate within the deformation bands, obtained with a diametral extensometer, approach 15-20/s. The localization of plastic flow into narrow, high velocity bands in this material is the result of the collective behavior of dislocations interacting at a high density. As demonstrated by TEM examination of the complex dislocation structures associated with these various events, however, it is difficult to rationalize a specific mechanism for these effects. One assumes that both serrated flow and the thermally activated strain bursts may occur in a number of different ways and hence the mechanism these observations pose a challenging problem for interpretation with models for the Portevin-LeChatelier effect in this material.

10:30 AM *BB4.6

Localized deformation commonly occurs during plastic flow of crystalline metals and leads to an evolution of microstructural patterning. One of the most widely observed examples is the lamellae microstructure associated with coarse slip, which can commence in the early stages of flow at strains on the order of 15% or less. We have shown that fine secondary slips, those that contribute significantly to the transition from stage 1 to stage 2 hardening, also play an important role in the nucleation, localization, and stabilization of bands of intense deformation. Within the framework of finetostrain crystal plasticity and using a hardening model that naturally predicts this transition (among other key behaviors of metallic single crystals), our calculations predict that these secondary slips are suppressed in the bands relative to the secondary-slip activity in the material outside of the bands. This gives rise to relatively softer response in the band, until eventually its hardening rate in stage 2 catches up with that in the matrix and the deformation stabilizes. For coarse slip, we have shown that these secondary slips can also control the thickness and spacing of bands, i.e. their patterning, as well as gradients of thickness across the bands and give rise to a more difficult crack growth problem. In addition, evidence suggests from related observations such as nanoindentation, locally elevated hardening due to the storage of geometrically necessary dislocations. To complete the model, incompatibility, as measured by a non-axisymmetric gradient of the dislocation density (the tensor field), is introduced into a nonlocal crystal plasticity theory.
but only in the instantaneous hardening relations. This theory preserves the classical bifurcation calculations that predict the onset of shear localization from a homogeneous state. Then, during localization, the effects on hardening of these gradients of secondary slip provide the mechanism that causes patterning.

11:00 AM BB4.7
AN ANALYSIS OF SHEAR-BANDING IN A C-Mn PIPE STEEL
Amie Benzing, Brown University, Div. of Engineering, Providence, RI; Jacques Besson, André Pinié, Ecole des Mines de Paris, Centre des Matériaux, FRANCE.

Plane strain tensile tests were carried out on specimens made of a C-Mn pipe steel. The specimens were cut in different orientations in the rolling plane at room temperature. A microscopic shear fracture mode was observed to develop macroscopically shear-like, as expected, whatever the specimen orientation. However, like in many structural materials, fracture starts after diffuse necking, at the center of the specimen, by microvoid coalescence giving rise afterwards to the macroscopic shear fracture mode. In this paper, the effect of coalescence on shear band development and on associated fracture mode in plane strain is analysed numerically. The calculations are performed using a recent elastic-viscoplastic Gurson-like model that accounts for void size evolution, coalescence and post-coalescence micromechanics along with isotropic hardening and orthotropic plasticity for the matrix behavior. The latter is introduced to represent the actual flow properties of rolled materials. No kinematic hardening nor necking formulation are used in order to focus attention on coalescence effects and to discuss, with respect to experiments, published results based on kinematic hardening and necking effects. The most important finding is the synergistic effects of plastic anisotropy and the post-coalescence yield surface curvature on the onset of a shear band after the fracture sets in at the center of the specimen.

11:15 AM BB4.8
DAMAGE, INSTABILITIES, AND SIZE EFFECT IN SUPERPLASTICITY
Hassan M. Zbib, Morgan B. Greenough [Taylor], Washington State University, School of Mechanical and Materials Engineering, WA; Moe Khaleel, Pacific Northwest National Laboratory, Richland, WA.

Superplastic forming is a valuable metal working technique because of the extreme ductility that can be achieved. However, it is limited in application due to the presence of small voids that grow and coalesce during the forming process often causing deformation instability, shear banding and premature failure. In order to understand and control this phenomenon accurate constitutive models must be developed which account for void parameters that affect the macroscopic behavior of the material. This work looks specifically at the effect of void size and spacing on the ductility and flow stress of viscoplastic materials. Based on the gradient-dependent theory of plasticity, a model is proposed that accounts for size effects by incorporating strain gradient terms into a continuum based constitutive equation. Both experimental testing and finite element modeling were performed on Pb-Sn, tensile specimens with small holes drilled in them in random patterns. The experimental tests indicate that a decrease in void size results in an increase in ductility. The FE results demonstrate that the gradient terms strengthen the material by diffusing the strain in areas of high strain concentration and delay failure by slowing void growth. In addition, the model predicted an increase in ductility and flow stress with decreasing void size.

11:30 AM BB4.9
HIGH SPEED IN OBSERVATIONS OF TRANSIENT HIGH TEMPERATURE VERTICAL MICROSTRUCTURES IN SOLIDS DURING ADIABATIC SHEAR BANDING
A.J. Bossis, G. Rawchandran and P.R. Guduru, Graduate Aeronautical Laboratories, California Institute of Technology, Pasadena, CA.

The structure of adiabatic shear bands in solids has been a subject of much interest and modeling, with very little independent experimental evidence. By using a unique infrared high-speed camera especially constructed for recording highly transient temperature fields at the nanosecond time scale, we are able, for the first time, to record the spatial and temporal microstructure with dynamically growing shear bands in metals. It is found that the temperature distribution along the band is highly non-uniform and possesses a transient, short range periodicity in the direction of shear band growth in the form of an array of intense ‘hot spots’, reminiscent of well known shear-induced hydrodynamic instabilities in fluids. This is contrary to the prevailing classical view which describes the deformations and the temperatures within the propagating essentially one-dimensional fields. The tip of a propagating shear band has been observed in real time for the first time and is found to possess a diffuse structure, with a gradual temperature increase.

SESSION BB5. DEFORMATION AND PATTERNING AT SMALL SCALE: MODELS AND EXPERIMENTS
Chair: D.W. Buehler, Turag A. Kuthai, Wednesday Afternoon, April 18, 2001
Golden Gate B1 [ Marriott]

1:30 PM BB5.1
SLIP BAND AND STEP FORMATION AROUND SMALL SCALE INTEMANDATIONS
D.F. Buehler, C.L. Woodcock, and K.R. Meckich; Mechanical and Materials Engineering, Washington State University, Pullman, WA.

Indentations in metals have traditionally been considered to be hemispherical zones of deformation surrounding a core region defined by the contact radius of the indenter tip. This has proven to be accurate in large scale indentations, but when indentation sizes reach length scales smaller than several microns the actual shape of the deformation pattern is dominated by the relationship between crystal orientation and the stress field surrounding the indentation. Additionally, as indentations are made with sharper tips, there are difficulties in tip calibration to accurately assess mechanical behavior. With the ability to image the surface around an indentation using scanning probe techniques, it is possible to characterize deformation in terms of localized dislocation formations such as slip steps around the indentations. The current study has been undertaken to examine if slip step formation is related to the plastic flow characteristics of the metal. A BCC titanium alloy which has been charged with hydrogen to levels of 140 and 2600 ppm H has been indented, and the resulting out of plane deformation in the surrounding surface has been identified. Slip steps with spacings between 50 and 300 nm were found surrounding the indentations. A decrease in the number of slip steps has been shown to correlate to a reduction in the out of plane deformation, which is controlled by the addition of hydrogen into the alloy. The height of the slip steps was also identified, and is not related to the step spacing. Models which consider remnant deformation characteristics around indentations as a method of identifying mechanical properties will be discussed.

1:45 PM BB5.2
THE FORMATION OF PRISMATIC LOOPS AND DISLOCATION PATTERNING DURING DEFORMATION
Patrick Veyssière, LEM, CNRS-ONERA, Châlons, FRANCE; Fabienne Grégoire, LPMi, Institut Galilée, Villeurbanne, FRANCE.

The formation of prismatic loops and the interactions of these with mobile dislocations is investigated in γ-TiAl deformed at room temperature in single slip by 1/2<110> dislocations. It is shown that loops usually originate from multiple cross-slip annihilation within the same dipole. These loops form in a planar way and, after a second cross-slip event, the loop then moves with the glide of the second screw dislocation. This second cross-slip event is then detected by a single cross-slip annihilation. This can be explained by multiple cross slip events. Experimental evidence in support of the above mechanisms is provided and the applicability of this model to simple metals is discussed. The observed annihilation of loop strings by a conservative process involving single impacting dislocation will be presented. In case of slip localization, as in metals with moderate stacking fault energy, this mechanism is believed to be responsible for a reduced accumulation rate in loop walls.

2:00 PM BB5.3
EXPERIMENTAL-COMPUTATIONAL CORRELATIONS OF DEFORMATION STRAIN GRADIENTS IN FCC-BASED Bi/CRYSTALS, Bimal K. Kulkarni, Roberto Garcia, University of California-San Diego, La Jolla, CA; Maks Kamek, Adam Schwartz, Lawrence Livermore National Laboratory, Livermore, CA; Paul Browning, Solar Turbines, San Diego, CA.

This work is motivated by the need to experimentally evaluate the mechanical response of model micrometeric bicrystals with a view to embedding such boundary characteristic responses into existing numerical models for polycrystal aggregates. Efforts are targeted to document the spatially resolved deformation strain gradient via high resolution e-beam lithography techniques, whereby ultrafine fiducial grids are deposited on polished test specimens, and monitored by SEM imaging at discrete loading steps. Current efforts are focused on directionally solidified bicrystals of Ni-base CMSX-10 alloy, each grown along [001], incorporating a 2.15 degree twist boundary. The bicrystals are strained up to 20% in compression, with the fiducial deformation patterns recorded at finite intervals. Results indicate that strain gradients in the vicinity of the boundary are principally
affected by i) the grain boundary misorientation, and ii) the specific orientation of the grain boundary plane with respect to the loading axis.

2:15 PM BB5.4
EVALUATION OF DISLOCATION STORAGE BY MEANS OF CRYSTAL PLASTICITY ANALYSIS. Tessya Ohashi, Kitami Institute of Technology, Dept. of Mechanical Systems, Kitami, JAPAN; Kumihisa Akaawa, Graduate Student, Kitami Institute of Technology, Dept. of Mechanical Systems, Kitami, JAPAN.

Plastic glide of metal crystals is carried by movement of dislocations. As a result of this, we usually observe an accumulation of dislocations in the crystal after plastic deformation. Dislocations that accompany successive plastic slip are called the geometrically necessary dislocations. So far, we have been analyzing slip deformation in the microstructures of F.C.C. type crystals, which contain some types of inclusions, and evaluate the accumulation of the geometrically necessary dislocations around them. In this paper, we analyze dislocation structures in microstructure models that include a cuboidal or spherical shaped inclusion. When the inclusion is cuboidal, we observe two types of dislocation structure, one corresponding to the Orowan loop and the other to the structure of kink wall. In the case of spherical inclusion, we observe the Orowan loop, kink wall structure, and some additional structures. We reconstruct images for dislocation structures from numerical data obtained by the crystal plasticity analysis, and discuss on the formation of the dislocation structures and stress state after constrained plastic slip around inclusions.

3:00 PM BB5.5
MICROMECHANICAL MODELING OF TWINNING. Wilfried T. Marquart, Institute of Mechanics, Montanuniversitaet Leoben, Leoben, AUSTRIA; Henryk Petryk, Polish Academy of Sciences, Warsaw, POLAND; Franz Dieter Fischer, Institute of Mechanics, Montanuniversitaet Leoben, Leoben, AUSTRIA; Fritz Appel, Helmut Clemens, Institute of Materials Research, GKSS-Research Center, Geesthacht, GERMANY.

Intermetallic $\gamma$ [TiAl] based alloys have been qualified to become important materials for advanced applications in aeronautic and aerospace industries. They offer an attractive combination of low density, good high-temperature strength and oxidation resistance. Research and development have progressed significantly within the last few years and led to a comprehensive understanding of the fundamental correlations between alloy composition, microstructure, processing behavior and mechanical properties such as strength, ductility, toughness, fatigue strength, and creep resistance. The mechanical properties are closely related to the slip and twinning characteristics of the L12 structure of $\gamma$ [TiAl]. The deformation of $\gamma$ [TiAl] under most conditions occurs on the slip planes of ordinary dislocations with the Burgers vector $b = 1/2[110]$ and superdislocations with the Burgers vector $b = 1/4[001]$. In the absence of superdislocations, there is one distinct twinning shear direction along $1/6[112]$ per $\gamma$ [TiAl] plane that does not alter the ordered L12 structure of $\gamma$ [TiAl]. There is growing evidence that in $\gamma$ [TiAl], as well as in other titanium aluminate alloys, the activation of glide systems involving superdislocations is difficult. Thus, upon straining of polycrystalline materials high constraint stresses can be developed between adjacent grains, which may lead to premature failure. However, under most conditions mechanical twinning can simultaneously operate with glide of ordinary dislocations and thus compensate for the lack of independent slip systems. The contribution of mechanical twinning to the kinetics and dynamics of deformation of $\gamma$ [TiAl] is not fully understood and will therefore be subject of the present study. In this contribution an energy-based description of twinning is presented. Conditions for a minimal and a maximal twin thickness as well as the minimum distance between twins are investigated applying an energy minimization criterion. Simulation results are compared with those derived from an analytical energy-based concept as well as with experimental results obtained from transmission electron microscopy investigations.

3:15 PM BB5.6
MICROSTRUCTURAL INTERFACIAL FAILURE INITIATION AND EVOLUTION IN CRYSTALLINE AGGREGATES. W.M. Ashby and M.A. Zikry, Department of Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, NC.

A multiple-slip dislocation-density based constitutive formulation and specialized computational schemes have been developed to characterize material failure on the appropriate physical scales needed for the accurate prediction of physical mechanisms that control failure initiation, growth, and coalescence. Dislocation-density transmission and blockage interfacial conditions and local stress fields have been obtained for grain-boundary distributions associated with random and tilt orientations. These evolving local stress fields are used as failure criteria to track the initiation and evolution of intergranular and transgranular fracture. The interrelated effects of grain boundary orientation, dislocation density pile-ups and evolution, geometrical and thermal softening, void distribution and geometry, and hydrostatic stresses on failure paths in cubic crystalline materials have been studied. Based on the present analysis and on comparison with experimental observations, it is shown transgranular and intergranular failure can be characterized in terms of the competition between the strengthening and the softening mechanisms of the crystalline structure.

3:30 PM BB5.7
AN ANALYSIS OF FATIGUE CRACK GROWTH USING DISCRETE DISLOCATION PLASTICITY. V. Deshpande, Brown University, Division of Engineering, Providence, RI; H.H.M. Greving, Delft University of Technology, Koiter Institute Delft, THE NETHERLANDS; A. Needleman, Brown Univ. Division of Engineering, Providence, RI; E. Van der Giessen, Delft University of Technology, Koiter Institute Delft, THE NETHERLANDS.

Cyclic loading of a plane strain mode I crack under small scale yielding is analyzed using discrete dislocation dynamics. A cohesive surface constitutive relation is specified so that crack growth emerges directly from the boundary value problem solution. Crack growth is found to occur under cyclic loading conditions even when the driving force is smaller than what is required for crack growth under monotonic loading conditions. Fatigue emerges in the simulations as a consequence of the evolution of internal stresses associated with the irreversibility of the dislocation motions rather than as a result of a specified phenomenological cyclic plasticity constitutive model. It is also found that the predicted onset of fracture is very sensitive to perturbations in the initial conditions.

3:45 PM BB5.8
MODELING OF DISLOCATION MOBILITY IN METALS: EFFECT OF OBSTACLES AND THERMAL PROCESSES. Tetsuo Hirata, Hussein M. Zbib, School of Mechanical and Materials Engineering, Washington State Univ., Pullman, WA.

Thermally activated dislocation glide velocity through point obstacle arrays is studied analytically and computationally. By techniques of statistical mechanics, the condition for the mechanical stability of dislocation lines held by point obstacles and the basic statistical properties such as the segment length distribution are derived. In the limit of weak obstacle strength, functional forms similar to the conventional Fredel relations are obtained but with different proportionality constants. The average flight velocity after an activation event as a function of stress and the temperature is estimated by the discrete dislocation dynamics (DD). This numerical calculation includes the effect of selfstress, interaction with electrons and phonons, and the inertia effect during collision with obstacles. These results are used to study the dislocation velocity in a wide range of parameter space of stress, temperature, the obstacle concentration, strength, etc. The obtained velocity vs. stress curves show both obstacle-controlled regions (non-linear stress dependence and viscous motion regions (linear stress dependence) in low and high stress regions, respectively. This result is in good qualitative agreement with available experimental data. Also special cases of low temperatures are investigated where the metals can be in a superconducting state. The results of the temperature dependence of the flow stress produced a sharp yield peak anomaly, indicating the strong coupling of the obstacle-controlled region with the viscous motion region through the inertial effect.