SYMPOSIUM BB

Material Instabilities and Patterning in Metals

April 17 – 18, 2001

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* Invited paper

SESSION BB1: DISLOCATION STRUCTURES & MECHANICAL PROPERTIES

Chairs: Darcy A. Hughes and Bennett C. Larson
Tuesday Morning, April 17, 2001
Golden Gate B1 (Marriott)

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, automated white-beam diffraction software, and newly developed depth-profiling techniques have made 3-D 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 orientation, phase, shape, and stress/strain 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.
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 Michigan, Lucent Technologies, and Howard University; the operation of the APS is sponsored by the DOE.

9:00 AM BB1.2

DISLOCATION WALLS IN FINITE MEDIA: THE CASE OF AN INFINITE SLAB. M.P. Surh 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-ranged 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 infinite 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 the 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 not transmit shear components of a dislocation stress field. In order to study the importance of boundary conditions, dislocation walls have been evaluated in a slab. 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 tilt walls possess 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. L.E. Levine, G.G. Long, R.J. Fields, NIST, Gaithersburg, MD.

New ultra-small-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 electron density variations within 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 imager. Changing q allows features at different length scales 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 cavities in polycrystalline Cu.

9:30 AM BB1.4

NANO-LAMELLAR STRUCTURES IN A ROLLED Cu-Ag ALLOY. M.T. Lyttle 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 ($\sim$20 nm) compared to those produced by the rolling of pure copper. Compared to the behavior of single-phase fcc metals, the average misorientation of Cu-Ag boundaries increases at a much more rapid rate. Rapid divergence of local crystal orientations leads to the early development of high-angle Cu-Ag interface misorientations, while less misorientation accumulation occurs within the individual copper and silver layers. With increasing deformation, orientations of the copper and silver phases in a single region are generally observed to diverge to two distinct textures.

9:45 AM BB1.5

LOCAL 3-D STRAIN AND ORIENTATION MEASUREMENTS IN TENSILE STRAINED AND NANOINDENTED COPPER USING X-RAY MICROBEAMS. Wenge Yang, B.C. Larson, G.E. Ice, J.Z. Tischler, J.D. Budai, K.-S. Chung, 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. Lowe, Howard University.

We have used submicron resolution broad band-pass (white) x-ray microbeams and a newly developed x-ray microscopy depth-resolution technique to determine the local orientation and strain/stress in deformed Cu crystals within volume elements $\sim$0.7 x 0.7 x 1.0 μm^3. 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 microbeams will be compared with TEM observations, and strain levels associated with the plastic/elastic deformation and dislocation walls in the tensile strained copper will be discussed. The measurements on nanoindented Cu were used to determine the spatial distribution of plastic deformation below the blade edge and flat face regions of Berkovich indents. Combinations of several lattice rotation systems were observed under the blade edge area, while nearly one-dimensional tilts 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, NT, 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 Hosson, Department of Applied Physics, Materials Science Center and Netherlands Institute of Metals Research, Nijenborgh, THE NETHERLANDS; Otmar Kanert,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 ionic crystals, i.e. pulsed nuclear magnetic resonance (NMR), that was introduced by us in the past. The method is essentially based on the interaction between nuclear electric quadrupolar moments and elastic-field gradients at the nucleus. The surrounding of a nucleus may affect NMR properties like relaxation time and accordingly NMR can be used to study the environment of the nuclei providing microscopic information of atomic motion. In contrast to in-situ transmission electron microscopic observations of dislocation motion, NMR detects more of the bulk of the material and does not allow only investigation of dislocations near free surfaces, like in TEM. There exist a large number of studies on the dynamics of point defects in metals induced by plastic deformation. The experiments, however, are usually performed on materials cold-worked at various temperatures. The paper will show that in-situ pulsed NMR is an excellent experimental method to scrutinize the actual kinetics involved. In this investigation we focus on plastic deformation experiments at strain rates up to 1 s-1. In particular, the paper will concentrate on the enhanced atomic diffusion under plastic deformation that was observed in aluminum and in ionic crystals. Evaluation of the data yields the actual concentration of the excess vacancies as a function of temperature, strain and strain rate. The findings are in agreement with a model that describes the formation mechanism of the vacancies and the annihilation process by the diffusion of vacancies to dislocations acting as vacancy sinks. The resulting dislocation structures are analyzed with transmission electron microscopy.

11:00 AM BB1.7
CONSTRAINTS ON SCALING OF THE DISTRIBUTION OF SPACINGS OF GEOMETRICALLY NECESSARY DISLOCATION BOUNDARIES. Maria Bartelt, Lawrence Livermore National Laboratory, Livermore, CA.

Transmission electron microscopy analyses [e.g., Hughes et al., Acta Mater. 48, 1897, 2985 (2000)] of several monotonically deformed pure metals find a “universal” form for the scaling function, g(D), for the distribution of spacings, D, between geometrically necessary dislocation boundaries (GNBs). In particular, the strain dependence is entirely folded into the average spacing, D*, and the expected fraction of spacings within a range of D depends only on D/D*. Under what (simple) rules does an arrangement of GNBs evolve in these systems that preserve such “universal” behavior? Observed short-range order in the GNB positions suggests that GNB spacings are not selected at random for new boundary formation. Motivated by this feature, a model for the evolution of g(D) was studied in which the probability of selection of a spacing scales with a power-law of the spacing value (thereby capturing the expected bias towards selection of wide spacings). In the model, the form of this probability controls the shape of g(D/D*), and constrains the strain evolution of D* (or, correspondingly, of the mechanical strength). Remarkably, the predicted constraint is satisfied by the experimental data, which in turn identify the power-law exponent. At higher strains, we allow for removal of boundaries due to coalescence. Interestingly, to first order in the (expected small) spacing of coalescing boundaries, the shape of g is insensitive to coalescence (due to cancellation of terms). For suitable choices of the sample geometric reduction factor, and the GNB spacing at coalescence, results from simulations of this model reproduce the observed distribution of spacings, and the basic strain dependence of the number of GNBs.
This work started at Sandia National Laboratories in collaboration with Darcy Hughes, with support from the USDOE-OBES under contract No. DE-AC04-94AL85000. At LLNL, this work was supported by the USDOE-ASCI under contract No. W-7405-Eng-48.

11:15 AM BB1.8
DISLOCATION BOUNDARIES AND SLIP SYSTEMS IN UNIAXIALLY DEFORMED <110> AL SINGLE CRYSTALS. Grethe Winther, Xiaoxu Huang, Soeren Faester Nielsen, John Wert, Materials Research Department, Risoe National Laboratory, DENMARK.

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 with these. 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. Both tensile deformed and uniaxially compressed aluminium single crystals are examined, i.e. the crystals have the same sets of slip systems operating in opposite directions. The deformation axis chosen is <110> in which case two sets of coplanar slip systems are predicted to be active. In both types of deformation the crystals break up into macroscopic bands hundreds of micrometers wide. In each band subsets of the four slip systems dominate. The deviation of the boundaries from the slip planes in different bands is correlated with the active 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 <112> and <110> deviation axes is discussed. These axes have previously been found in tensile deformed copper single crystals of other orientations and in tensile deformed polycrystalline aluminium 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'Héres, FRANCE.

A statistical analysis of the acoustic emissions induced by dislocation motion during the viscoplastic deformation of ice is presented. The recorded acoustic waves provide an indirect measure of the inelastic energy dissipated during dislocation motion. Creep as well as controlled strain-rate experiments indicate that collective dislocation dynamics during viscoplastic deformation is a complex, intermittent and inhomogeneous process characterized by avalanches in the motion of dislocations. These dislocation avalanches consist of a mainshock correlated in time with a sequence of few aftershocks. These avalanches are themselves uncorrelated in time. The distribution of avalanche sizes, identified with the acoustic wave amplitude (or the acoustic wave energy), is found to follow a power law. This indicates that collective dislocation motion is a scale-free phenomenon strongly out of equilibrium. These results suggests therefore that viscoplastic deformation in ice and possibly in other materials could be described in the framework of non-equilibrium critical phenomena.

11:45 AM BB1.10
RELATIONSHIP BETWEEN MICROSTRUCTURES AND CONSTITUTIVE BEHAVIOR OF A SERIES OF TEMPERED MARTENSITIC STEELS. Philippe Spätig, Robin Schäublin, Max Victoria, Fusion Technology-CRPP-EPFL, Villigen PSI, SWITZERLAND.

The constitutive behavior and the microstructures of a series of 9Cr ferritic/martensitic steels, which are leading fusion reactor structural candidate materials, are investigated. Since there is a lack of systematic studies of the effects of microstructures resulting from the heat-treatment and the composition on the constitutive behavior, a comparison of the mechanical properties in relation to the microstructures of different steels, with various contents of W, V, Ta, Mn, Si and N and heat treatment, is presented. The mechanical properties are investigated by means of tensile tests as well as compression experiments allowing to reach larger strains. The plain tensile tests are supplemented with Cottrell-Stokes type tests to investigate the temperature and plastic strain dependence of strain. The testing is carried out over a domain ranging from 80K up to 723K. Flow stress decomposition and strain-hardening stages are proposed. The microstructures of the undeformed materials are characterized by transmission electron microscopy (prior austenite grain size, carbide distribution, initial dislocation density) and are also investigated at different strain levels along the deformation curves. Their relationship to the strain-hardening is discussed. It must be noted that these steels undergo the usual ductile to brittle transition in lowering temperature and that this paper aims at better understanding the basic constitutive behavior in this transition fracture regime. Ultimately, these constitutive behaviors are used as input for FEM simulations of fracture properties.

SESSION BB2: MULTISCALE MODELS, SIZE EFFECTS AND STRAIN GRADIENT THEORIES

Chairs: Lyle E. Levine and Hussein M. Zbib
Tuesday Afternoon, April 17, 2001
Golden Gate B1 (Marriott)

1:30 PM *BB2.1
STRAIN PERCOLATION THEORY AND ITS APPLICATION TO DEFORMATION IN METALS. Robb Thomson (Retired), Lyle Levine, NIST, MS&E Laboratory, Gaithersburg, MD; Y. Shim, University of Georgia, Center for Simulational Physics, Athens, GA.

We have developed a percolation model for the fine slip which occurs at all stages of deformation in metals. In extensive exploration of the mathematics of the model, we have shown that both the geometrical and strain variables belong to the same universality class as ordinary percolation theory. A straining sample is shown to be a self organizing system, with the model in the slightly super critical regime, and a generic, universal stress-strain law can be derived. In applying the model to real materials, however, it is necessary to account for the localization of the fine slip lines into the gross slip bands observed in stages II and III. In addition, the strain occurs in punctuated bursts, with significant relaxation periods between bursts. And finally, it is observed that the dislocation structures group into two different classes of boundaries labelled GNB's and IDB's. We will discuss the kinds of amendments which must be incorporated into the model in order to account for these observations.

2:00 PM BB2.2
DISLOCATION PATTERN FORMATION - SIMULATIONS OF ANNEALING IN TWO DIMENSIONS. Nathan Argaman, Dept of Physics, NRCN, Be'er Sheva, ISRAEL.

A two-dimensional discrete dislocation dynamics code was developed and used to simulate dislocation patterning. For the present study, simulations with both glide and some climb allowed were chosen. In these circumstances patterning takes place even in the absence of external stresses or dislocation sources. A triangular underlying lattice was assumed, with the three slip systems equally populated initially. Well-defined dislocation walls and cells are observed to form from random initial conditions. The structure coarsens with time, i.e. the 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 multiscale approach, a new simulation methodology is suggested, in which the discrete moving objects are dislocation wall segments rather than individual dislocations. The most important rule governing the dynamics of the dislocation walls is local conservation of the net Burgers' 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. Shim[1,2], L.E. Levine[2], R. Thomson[2]. [1]Center for Simulational Physics, University of Georgia, Athens, GA. [2]MS&E Laboratory, National Institute of Standards and Technology, Gaithersburg, MD.

Using a simple 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 standard 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 self-organize 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 asymmetric bell-shape function. Other critical aspects of the model are also discussed.

2:30 PM BB2.4
A PHASE-FIELD THEORY OF DISLOCATION 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 Spatiales, Liège, BELGIUM.

A phase-field theory of dislocation dynamics, strain hardening and hysteresis in ductile single crystals is presented. Specifically, we consider the motion of large numbers of dislocations within discrete slip planes through random arrays of point obstacles under the action of an applied shear stress. 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, bow-out, pinching, and the formation of Orowan loops. The theory predicts a range of behaviors which are in qualitative agreement with observation, including: hardening and dislocation multiplication in single slip under monotonic loading; Taylor scaling, both under monotonic loading and, in an appropriate rate form, under cyclic loading; the Bauschinger effect under reverse loading; the fading memory effect, whereby reverse yielding gradually eliminates 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 Atomico 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 visualisation, energy calculations and local crystalline order. Grain boundaries are essentially similar to those found at the micron-scale, i.e similar structural units are found, providing evidence against the view of grain boundaries in nano-crystals as liquid-like interfaces. Modelled samples are deformed by constant uniaxial tensile stress. A change in deformation mechanism is observed: at the smallest grain sizes all deformation is accommodated in the 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 intragrain dislocation activity is observed. In this paper we address the microscopic view of sliding. When a homogenous 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, some of them reaching the critical conditions to pass its saddle point 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 emitted from the grain boundaries are discussed and their relative importance as function of grain size and grain misorientation are determined.

3:30 PM *BB2.6
DISLOCATION, GRADIENTS, AND SIZE EFFECTS. Elias C. Aifantis, 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 MICROMECHANICAL 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 generation of deformation 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 macroscopic deformation. The dislocation structures are deduced from the plastic deformation gradient field by recourse to Kroner's formula for the dislocation density tensor. The theory is rendered nonlocal by the consideration of the self-energy of the dislocations. Selected examples demonstrate the ability of the theory to: predict the full set of dipolar walls which are observed to arise 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 POLY-CRYSTALS. Dilip Chandrasekaran, Kjell Pettersson, Dept of MS&E, Royal Institute of Technology, Stockholm, SWEDEN.

The strengthening effect of grain boundaries is well established and observed experimentally as the Hall-Petch relationship. In this paper the mechanisms for the observed Hall-Petch effect 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 capabilites are evaluated. The focus is towards deformation at small strains and specifically the onset of plastic deformation, with special attention devoted towards the specific role of grain boundaries. The fundamental implications of the different approaches are discussed with reference to two different classes of materials; -Materials with locked dislocations (e.g. steels) -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 revealing aspects of localized flow 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 that illustrate the development of plastic deformation in localized bands, such as during bending of a single crystal, and we analyze their spacing. Also we present results of simulations where interfaces provide barriers to slip. The associated boundary effects induce a length scale and we investigate to what extent these can be described by gradient-type continuum theories.

SESSION BB3: POSTER SESSION DEFORMATION AND PATTERNING AT SMALL SCALE: MODELS AND EXPERIMENTS

Chair: Hussein M. Zbib
Tuesday Evening, April 17, 2001
8:00 PM
Salon 1-7 (Marriott)

BB3.1

MACROSCOPIC SHEAR BANDING IN AN ALUMIUM-BASED ALLOY DURING EQUAL-CHANNEL ANGULAR PRESSING.

Jingtao Wang , Yuzhong Xu, Lizhong Wang* and Haibo Wang, School of Metallurgy, 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 ultrafine structures. It is generally considered that the deformation is homogeneously distributed in materials after ECA pressing. The present investigation shows, however, that severe macroscopic shear band, which extends from bottom to upper surface and slants to the longitudinal axis of specimen at an angle of 45 degree, develops at regular intervals. The deformation-banding behavior is strongly affected by different ECA pressing routes. With routes A and B, macroscopic shear banding occurs in regular intervals, while with route C no serious macroscopic shear banding was observed.

BB3.2

INSTABILITY OF BUCKLING PATTERNS: FROM STRAIGHT-SIDED TO WORMLIKE STRUCTURES.

F. Cleymand, J. Colin, C. Coupeau, J. Grilhé Poitiers University, Futuroscope, 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 stresses, 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 stresses favourable to the waving of straight-sided blisters.

BB3.3

A GENERALIZED MODEL OF THE YIELD DROP IN IMPURE SEMICONDUCTORS.

Boris Petukhov, 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 Alexander-Haasen model of the avalanche dislocation multiplication, qualitatively good, does not describe some features of the phenomenon, for example, the great difference in behavior of Czochralski and floating zone-grown crystals. To account for such difference, it is natural to ascribe it to the dynamic interaction between impurity atoms and moving dislocations, and to incorporate this interaction into the model of the yield drop. This contribution presents a combined approach, which unites the dislocation multiplication model and modified dynamic strain aging model, specific for the dislocation motion by the kink mechanism. New insight into the problem of the elastic-plastic transition is achieved, and a generalized description of the yield drop phenomenon for impure semiconductors is suggested, which is compared with experimental data.

BB3.4

DEFORMATION INSTABILITIES IN BULK AMORPHOUS ALLOYS.

Elena Tabachnikova Institute for Low Temperature Physics & Engineering, Kharkov, UKRAINE; Michael Macht, Hahn-Meitner Institut, Berlin, GERMANY; Josef Miskuf, Kornel Csach, Institute of Experimental Physics, Kosice, SLOVAKIA.

Unstable character of plastic deformation is typical not only of crystalline materials but also of novel class of materials - bulk metallic glasses. Mechanisms of deformation and failure have been studied on the $Zr_{46.8}Ti_{8.2}Cu_{7.5}Ni_{10}Be_{27.5}$ bulk amorphous alloy. Samples 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 jump-like character. Plastic deformation realizes by localized glide bands. Mean amplitude of jumps corresponded to the plastic deformation of 0.03%. Localized glide bands were observed with the TESLA BS-340 scanning electron microscope as steps at the side surface of deformed cylindrical specimens. The failure of samples at all studied temperatures took place by the ductile shear failure mode through the adiabatic catastrophic shear. Samples were fragmented in two parts by sliding along the surface, which was oriented approximately at 45 deg. to the compression axis. Obtained results are analyzed in the framework of notions on a polycluster structure of amorphous alloys and dislocation motion along intercluster boundaries.

BB3.5

THE INTERACTION OF A CIRCULAR DISLOCATION PILE-UP WITH A SHORT RIGID FIBER: A 3-D DISLOCATION DYNAMICS SIMULATION.

Tariq A. Khraishi, Department of Mechanical Engineering, University of New Mexico, Albuquerque, NM; Hussein M. Zbib, School of Mechanical and Materials 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 might arise in metal-matrix composites, for example. Here, given 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. For proper interaction, one needs to impose the correct boundary condition for the problem. This condition is that of zero elastic displacements on the fiber's surface. The enforcement of such a boundary condition is done numerically at collocation points on the surface (the more the better, covering the whole surface in the limit). Here, the elastic displacements at the surface collocation points due to the displacement field of the circular dislocation pile-up surrounding the fiber are annulled by a distribution of N rectangular dislocation loops (each with three Burgers vector components) situated at or near the fiber's surface. Our problem thus reduces to finding the set of 3N unknown loop Burgers vector components which will collectively annul the displacements at the surface of the rigid fiber stemming from the circular pile-up. The formulation calls on the solution of a $3N \diamond 3N$ system of linear algebraic equations in order to determine the sought after Burgers vector components. Once these Burgers vectors are determined, the Peach-Kohler (PK) force that the pile-up senses due to the presence of the fiber, and emulating its influence, can be straightforwardly calculated. Finally, knowing the PK force distribution and using a suitable kinetic model for the glide velocity of dislocations, the dynamic arrangement and equilibration of the circular dislocation pile-up follows suit from the use of a simple time marching scheme.

BB3.6

STABILITY OF DISLOCATION SUBSTRUCTURES AT DEFORMATION TEMPERATURE VARIATION AND MECHANICAL PROPERTIES OF TITANIUM IN RANGE 4.2-373 K.

V.A. Moskalenko, A.R. Smirnov, V.N. Kovaleva, B. Verkin Inst. 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 interacting 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 type of deformation-induced substructure. Stability of structural 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 alpha-titanium. One of them (at low temperatures below 160 K) presents chaotic-distributed straight segments of screw dislocations, they play role of background for a rising twin layers at deformation >2%. 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 strength characteristics (yield strength, true rupture stress) at room and higher temperatures, which is result of high stability of twin layers (main element of substructure) relatively to deformation temperature changing. Other type deformation-induced substructure is formed at temperatures above 180 K. Space ordered dislocation assemblages - reorientation bands are principal element of this substructure. Consisting of quasi-periodic walls of edge dislocations of the opposite sign reorientation bands are unstable during subsequent deformation at low temperatures (below 100 K) that is result of high mobility of edge dislocations. Therefore, predeformation-induced substructure of this type has not sufficient hardening influence on mechanical properties of titanium at low temperatures.

BB3.7

DUCTILE CATASTROPHIC SHEAR FAILURE THROUGH ADIABATIC SHEAR BANDING UNDER UNIAXIAL COMPRESSION OF NANOSTRUCTURED TITANIUM, MANUFACTURED BY SEVERE PLASTIC DEFORMATION. Vladimir Bengus, Institute for Low Temperature Physics & Engineering, Kharkov, UKRAINE; Josef Miskuf, Kornel Csach, Institute of Experimental Physics, Kosice, SLOVAKIA; Vladimir Stolyarov, Ruslan Valiev, 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 mcm 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% at 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 degree 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 localized 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" is considered as indirect indication of extreme local heating during ductile shear failure of nanostructured Ti. Probably similar phenomenon was observed by H.G.F. Wilsdorf and D.D. Makel in polycrystalline alloy Ti-8wt%Mn under tension (Scr. Met., 1987, v.21, p. 1229). 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 following non-uniform local adiabatic heating in the catastrophic shear band. Similarity of observed phenomenon to the ductile shear failure of metallic glasses allows to suppose that micro mechanism of a ductile shear failure in nanostrtuctured Ti is similar to that in metallic glasses and consists in avalanche shear spreading by grain boundary dislocations in nanostructured Ti.

BB3.8

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 are nearly planar dislocation boundaries that separate regions of different slip thereby accommodating the resulting mismatch in lattice rotations. 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 axis and boundary normal, which can be deduced from transmission electron microscopy (TEM) using Kikuchi pattern analysis. In the present study, misorientation axis and boundary normal are determined from TEM, and this experimental data is used as input to Frank's formula, giving three sets of dislocations 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.

BB3.9

THE CALCULATION OF ENERGETICAL PROFILE OF THE SHEAR IN THE ALLOYS WITH THE SUPERSTRUCTURE D019. Michail A. Baranov, Veronika V. Romanenko, Evgenya V. Chernyh, Michail D. Starostenkov, General Physics Dept, Altai 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 examples of the alloys Mg_3Cd and Ti_3Al. The interaction between atoms in the alloys is given by the sets of pair semiemperic interatomic potentials, besides the connections of A-B type are described by the potential, taking into account the anisotropy of crystal lattice of hcp. At the orientation of shears in bicrystals in the directions <21-30>, $< 10 - 10 >$ the potential profiles appear to be different. Two quasi periods, corresponding to the shear of semicrystals from 0 to -a0/2 <21-30> and from 0 to a0/2 <21-30>, were a0 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 plastic deformation 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.

BB3.10

MICROMECHANISMS OF PLASTIC FLOW LOCALIZATION AND FRACTURE IN SOLIDS. Valery. P. Kisel, Institute 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 is the same as for the stresses to initiate the first microcrack and macrocrack, 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 crystal shape-changes under loadings. The characteristics of cross-slip and climb processes correlate with proper structures of fracture surfaces and explain the brittle- to-ductile transition. In some cases the precursor deformation effects (due to generation of matrix defects) before fracture may be so 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 offen observed at different levels of the flow stress in standard materials.

BB3.11

MODES OF PLASTIC DEFORMATION AND MICRO-STRUCTURAL EVOLUTION. Valery P. Kisel, Inst. of Solid Sate 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 (SB), 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-spacings in slip bands, walls, LAGB, etc., thus transforming the LAGB into high-angle grain boundaries (HAGB) up to twinned, nanocrystalline, then amorphous structures, fracture and damage. The scaling behaviour of the reciprocal dependences of grain sizes, spacings of twins and SB, mean dislocation paths and their spacings in SB, walls, grain interior and L/HAGB, nanostructures of heavily deformed up to fracture versus the applied stress strongly confirms the universality of dislocation mechanisms of all deformation modes at atomic-/meso- and macroscopic scale lengths for various crystal classes, processings 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 temperature, stress and stress rate ranges (up to the shock wave stresses), for crystalline and disodered materials, etc.

SESSION BB4: DEFORMATION PATTERNING AND LOCALIZATION

Chairs: Geoffrey H. Campbell and Maximo Victoria
Wednesday Morning, April 18, 2001
Golden Gate B1 (Marriott)

8:30 AM *BB4.1

ROLE OF MICROSTRUCTURE IN PLASTIC FLOW LOCALIZATION. B.N. Singh[a] and S.J. Zinkle[b]. [a]Materials Research Dept, Riso National Lab, Roskilde, DENMARK. [b]Metals and Ceramics Div, Oak Ridge National Laboratory, Oak Ridge, TN.

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 a sudden yield drop followed by negative work hardening and may suffer from 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 particularly in the neutron irradiated materials has been a matter of serious concern regarding their application in structural components of fission and fusion 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 processes involved in the initiation and propagation of the flow localization has remained unclear. With the aim of clarifying the origin and ensuing consequences of the flow localization, first of all a critical review of the relevant experimental observations will be presented. These observations will be analysed in terms of the available theoretical models and the results of computer simulations of interaction between dislocations and irradiation induced defect clusters/loops. Finally, the main conclusions emerging from these evaluations will be summarized.

9:00 AM BB4.2

RADIATION HARDENING AND PLASTIC INSTABILITY IN NEUTRON IRRADIATED METALS AND ALLOYS. Dan Edwards, Pacific Northwest National Laboratory, Richland, WA; Bachu Singh, Risö 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 attempts been made 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_irr < Stage V) where hardening is due to the presence of finely dispersed, nano-size defect clusters. Under cascade damage 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 glissile 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 of rafts of dislocation loops, patterned arrays of defects, and more importantly from the standpoint of hardening, they can decorate 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 CuCrZr, 304 and 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-type obstacles to dislocation motion (Dispersed Barrier Hardening), and the other considers the possibility of the pinning of dislocation sources (Cascade-Induced Source Hardening).

9:15 AM BB4.3

ATOMISTIC INSIGHT INTO PLASTIC FLOW LOCALIZATION IN IRRADIATED METALS. Brian D. Wirth 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 high local strains, but overall specimen failure occurs at low uniform ductility and total strain. Plausible explanations for flow localization in irradiated face centered cubic metals involve the absorption of individual vacancies from stacking fault tetrahedra by gliding dislocations and dislocation cross-slip. However, a concise atomistic 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 jogged dislocations. The simulations are performed using embedded atom method interatomic potentials and provide atomistic insight into the mechanisms responsible for flow localization in irradiated metals. This work is performed under the auspices of U.S. Department of Energy and Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

9:30 AM BB4.4

DEFORMATION MICROSTRUCTURE EVOLUTION IN SINGLE CRYSTAL ALUMINUM. Michael F. Savage, Donald E. Kramer, Lyle 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 deformation microstructures in Al have focused primarily on cold-rolled polycrystalline material. In this study, the slip line evolution and underlying deformation 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 foils ex-situ, by Transmission Electron Microscopy. Relationships between the observed surface structures and the presence of Geometrically Necessary Boundaries (GNB's) and Incidental Dislocation Boundaries (IDB's) 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-Cr-Fe ALLOY (INCONEL). Harry N. Jones, C.R. Feng, Naval Research Laboratory, Materials Science and Technology Division, Washington, DC.

Nickel based alloys with nominal compositions similar to 78Ni -15Cr -7Fe, commonly referred to as 'Inconel', exhibit serrated flow (Portevin-LeChatelier effect) in the temperature interval of 230-730°C. Within this temperature range a complex series of thermally activated processes can also be observed when a wire sample of the alloy is heated with the direct resistance method under dead weight loading when stressed above the room temperature yield. These processes 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 at odds with models for the thermal activation of plastic flow in metals. As the temperature is increased after this first arrest a cascade of two or three large plastic instabilities involving the high velocity propagation of narrow deformation bands is observed. Measurements of the band velocity using the time of flight within a 50.8 mm gage length extensometer indicate that the velocity approaches 2.5 m/s in some cases. Estimates of the local 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 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. If one assumes that both serrated flow and the thermally activated strain bursts are manifestations of the same basic mechanism these observations pose a challenging problem for interpretation with models for the Portevin-LeChatelier effect in this material.

10:30 AM *BB4.6

A MODEL OF PATTERNING OF LOCALIZED PLASTIC FLOW. John L. Bassani, Dept. of Mechanical Engineering and Applied Mechanics, Philadelphia, PA.

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 lamella microstructure associated with coarse slip, which can commence in the early stages of flow at strains on the order of 10-3 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 finite-strain 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 follows. Gradients of these slips across the band give rise to lattice incompatibility and, as evidence suggests from related observations such as nano-indentation, locally elevate hardening due to the storage of geometrically-necessary dislocations. To complete the model, incompatibility, as measured by a skew-symmetric gradient of the lattice distortion (a third-order 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.

Amine Benzerga, Brown University, Div of Engineering, Providence, RI; Jacques Besson, André Pineau, 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. The macroscopic fracture mode was found to be 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 micro–void 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 shape evolution, coalescence and post–coalescence micromechanics along with isotropic hardening and orthotropic plasticity for the matrix behaviour. The latter is introduced to represent the actual flow properties of rolled materials. No kinematic hardening nor nucleation 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 nucleation 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 SUPER-PLASTICITY.

Hussein M. Zbib, Meagan 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 defromation 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 IR OBSERVATIONS OF TRANSIENT HIGH TEMPERATURE VORTICAL MICROSTRUCTURES IN SOLIDS DURING ADIABATIC SHEAR BANDING.

A.J. Rosakis, G. Ravichandran 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 microscale, we are able, for the first time, to reveal the spatial and temporal microstructure within 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 shear bands as being 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

Chairs: David F. Bahr and Tariq A. Khraishi
Wednesday Afternoon, April 18, 2001
Golden Gate B1 (Marriott)

1:30 PM BB5.1

SLIP BAND AND STEP FORMATION AROUND SMALL SCALE INDENTATIONS.

D.F. Bahr, C.L. Woodcock, and K.R. Morasch; 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 an 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 the 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, Chatillon, FRANCE; Fabienne Grégori, LPMTM, Institut Galilée, Villetaneuse, 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. This forms loop strings characterised by the property that the origin of a given loop is aligned in the screw direction with the end of one of its nearest neighbour loops. Rather than sweeping the loops, an impacting dislocation is captured in the string where it can be eventually annihilated by an incident dislocation with opposite sign forming a second string interspersed within the original string. By repetition of this process, a loose shoal of prismatic loops is built up whose ability to capture a further incoming dislocation increases with the number of strings accumulated. Experimental evidence in support of the above mechanisms is provided and the applicability of these to simple metals is discussed. If time allows, a manoeuvre for the annihilation of loop strings by a conservative process involving one single impacting dislocation will be presented. In case of slip localisation, as in metals with moderate stacking fault energy, this manoeuvre is believed 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 Kad, Roberto Garcia, University of California-San Diego, La Jolla, CA; Mukul Kumar, 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 misoriented bicrystals with a view to embedding such boundary characteristic responses into existing numerical models for polycrystal aggregates. Efforts are tailored to documenting 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 upto 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. Tetsuya Ohashi, Kitami Institute of Technology, Dept of Mechanical Systems, Kitami, JAPAN; Kazuhisa Asakawa, 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 that, we usually observe an accumulation of dislocations in the crystal after plastic deformation. Dislocations that accompany spatial gradient of the plastic slip strain 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. Marketz, 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 for Materials Research, GKSS-Research Center, Geesthacht, GERMANY.

Intermetallic γ(TiAl) based alloys have been qualified to become important materials for advanced applications in aeroengine 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 $L1_0$ structure of γ(TiAl). The deformation of γ(TiAl) under most conditions occurs on {111} planes by glide of ordinary dislocations with the Burgers vector b=1/2<110] and superdislocations with the Burgers vector b=<101] and b=1/2<11$\bar{2}$], respectively. Additionally, there is one distinct twinning shear direction along 1/6<11$\bar{2}$] per {111} plane that does not alter the ordered L10 structure of γ(TiAl). There is growing evidence that in (α_2 - γ) titanium aluminide 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 kinematics and dynamics of deformation of γ(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. Ashmawi 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.

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AN ANALYSIS OF FATIGUE CRACK GROWTH USING DISCRETE DISLOCATION PLASTICITY. V. Deshpande, Brown Univ. Division of Enginnering, Providence, RI; H.H.M. Cleveringa, Delft University of Technology, Koiter Inistitute Delft, THE NETHERLANDS; A. Needlleman, Brown Univ. Division of Enginnering, Providence, RI; E. Van der Giessen, Delft University of Technology, Koiter Inistitute 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.

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MODELING OF DISLOCATION MOBILITY IN METALS: EFFECT OF OBSTACLES AND THERMAL PROCESSES. Masato Hiratani, Hussein M. Zbib, School of Mechanical and Materials Engineering, Washigton 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 Friedel 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 self-stress, 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.