SYMPOSIUM Y

Influences of Interface and Dislocation Behavior on Microstructure Evolution

November 27 – 30, 2000

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*Invited paper
SESSION XI: INTERFACE MOTION I - COLLECTIVE GRAIN MOTION

Chair: Mark D. Asta and Andrew Rollett
Monday Morning, November 27, 2000
Independence E (Sheraton)

8:30 AM *Y13

INTERFACE DYNAMICS: A NOVEL TOOL FOR MICRO-STRUCTURAL CONTROL. Glimmer Gottstein, Dmitri A. Morosov, and V. V. Vvedensky (Max-Planck-Institute for Metal Research, Stuttgart, Germany). GERMANY. Luis S. Swiderski, Institute of Solid State Physics, Russian Academy of Science, Chernogolovka, RUSSIA.

The interface motion phenomena recrystallization and grain growth are processes with major impact on microstructure development and thus material properties. Interface migration is the key mechanism of these processes, and microstructure evolution can be biased through surface tension effects in a controlled and effective manner. We will present evidence that it is possible to affect the motion of grain boundaries by a variety of externally controlled driving forces. Although these effects cause major and adjustable changes of boundary motion, besides the well-known chemical effects like impurity drag the coupling of boundary migration with magnetic and elastic fields will be addressed. Moreover, we will discuss the role of processing parameters like temperature or pressure on mechanism with special attention will be given to the role of dislocation-boundary interaction which is a key issue in recrystallization. Finally, the consequences of boundary connectivity in terms of grain boundary networks with triple lines and quadruple junctions will be taken into account.

9:00 AM *Y1.2

GRAIN BOUNDARY MOTION IN POLYCRYSTALLINE MATERIALS. J. K. Forrer, N. R. Woodruff, University of Minnesota, Dept. of Chemical Engineering and Materials Science, Minneapolis, MN; J. R. Michael, Sandia National Laboratory, Albuquerque, NM; C.B. Carter, University of Minnesota, Dept. of Chemical Engineering and Materials Science, Minneapolis, MN.

Grain mass transport across grain boundaries in polycrystalline materials controls the densification process during sintering. In the case of liquid-phase sintering, a liquid film is present at the grain boundaries, which results in enhanced mass transport between grains. In this study, electron backscattered diffraction (EBSD) is used to obtain orientation information from glass-coated single-crystal alumina sintered to polycrystalline alumina. The glass in the grain boundary is a glassy phase of CaAl2Si2O7, which forms a liquid during sintering and provides a system to study mass transport across boundaries containing a liquid. EBSD patterns, taken from grains near the sintered interface, are used in conjunction with the original interface location to correlate mass transport across the grain boundary with the boundary orientation. EBSD patterns are also taken from the migrated region to study the orientation relationship of portions of the crystal through which the boundary migrates. These patterns indicate that there may be small-angle misorientations in the migrated regions. The misorientations may then be used to further study the driving force of the boundary migration mechanism.

9:15 AM *Y1.3

THE EFFECT OF INTERFACIAL FREE ENERGIES ON THE STABILITY OF MICHAELMASITES. A.C. Lewis, A.B. Muan, D. Van Heerden, T.P. Weils, Johns Hopkins University, Dept. of MSE, Baltimore, MD; D. Josell, National Institute of Standards and Technology, Gaithersburg, MD.

Laminated composites with polycrystalline layers typically break down at high temperatures through grain boundary growth and the pinchoff of individual layers. Such samples, when exposed to high temperatures, develop surfaces where boundaries meet the interfaces between layers. The depths of the grooves are controlled by the ratios of grain boundary and interfacial free energies, γ_b/γ_{int}. If γ_b is much smaller than γ_{int} there is little growth at grain boundary interfaces and the layering is stable. If γ_b is comparable to or larger than γ_{int} then there is significant grooving where grain boundaries meet the interfaces between layers. Depending on the dimensions of the grains, these grooves can extend through the entire layer, causing pinchoff at the grain boundary. This pinchoff destroys the layering and eventually leads to a gross coarsening of the microstructure. When one of the layers in the microcomposite is designed to have a specific resistance the microcomposite is extremely detrimental to the material's mechanical performance. Because microstructural stability is thus critical to performance, the ability to understand and predict the stability of microcomposites is a necessary tool. An existing model for the elimination of driving forces from requirements on free energies, γ_b and γ_{int}, as input parameters. Both biaxial and uniaxial zero creep tests have been used in conjunction with a transmission electron microscopy to measure these interfacial energies in Ag/Al and Nb/Nb3Si microaluminates. The measured energies are then used to explain the onset of instabilities and the eventual breakdown of layering in Ag/Ni multilayers and Au/Au substrates as well as in free-standing Nb/Nb3Si microaluminates.

10:00 AM *Y1.4

MODELING THE FORMATION OF GRAIN BOUNDARIES VIA COLLISION AND THEIR SUBSEQUENT EVOLUTION USING A PHASE FIELD METHOD. J. A. Warren, Alexander Lobkovsky, National Institute of Standards and Technology, Gaithersburg, MD; Ryo Kobayashi, Hakkaido University, Sapporo, JAPAN; W. Craig Carter, Massachusetts Institute of Technology, Cambridge, MA.

We present a new model of the solidification of whisker-oriented grains, their impingement, and the subsequent evolution of the resulting grain structure. This model is relatively simple to implement, contains a great deal of the relevant physics (including grain-boundary and liquid-solid interface energy anisotropy), misorientation dependent grain boundary energies, and the transition from wet to "dry" grain boundaries. The model is extensible to 3D and the inclusion of additional thermodynamic parameters is straightforward.

10:30 AM *Y1.5

MEOSCALE SIMULATION OF GRAIN GROWTH. David Kundeiner, Florin Manoleche, Irene Livasidis, Skimo Tassignon, Department of Mathematical Sciences, Carnegie Mellon University, Pittsburgh, PA.

The simulation of curved driven growth in grain boundary systems is becoming an important tool in understanding the behavior of microstructure evolution and there is much distinguished work in this subject. Here we address the mesoscale simulation of large systems of grain boundaries subject to the Mullins equation of curvature driven growth with the Herring force equation imposing triple junctions. We discuss several novel features of our approach which we anticipate will render it a flexible, scalable, and robust tool to aid in microstructural prediction. At present the results are for two-dimensional configurations. In this type of simulation, from our viewpoint the problem becomes one of solving a large system of evolution equations subject to complementing boundary conditions. It is metastable but always dissipative. In our technique we are able to track large numbers of grain boundaries (e.g., 20,000) by simulating the evolution of the network of curves constituting grain boundaries, a data structure an order of magnitude smaller than that of the grains themselves. A number of algorithmic innovations enhance both accuracy and speed. What is the result of the simulation? We discuss what such a simulation is capable of predicting, taking as an example the history of relative area population as it changes through the simulation. We do not use this data to seek the best distribution, like Hiller, Rayleigh, or lognormal, for a discussion see [6]. Instead we treat the set of distributions as the solution of an inverse problem for a time varying function and apply methods of optimization theory to determine the equation they satisfy. Even so, this leads to fundamental questions concerning the predictability of systems of large metastable systems. [6] Mullins, W. W. (1998). "Grain growth of uniform boundaries with scaling." Acta materials 46(17): 6123-6129.

11:00 AM *Y1.6

SIMULATION OF GRAIN GROWTH IN ALUMINUM FOIL USING EXPERIMENTALLY DERIVED BOUNDARY PARAMETERS. A.D. Rollett, C.C. Yang and W.W. Mullins, Carnegie Mellon University, Pittsburgh, PA.

Determining grain boundary energies and mobilities as a function of their crystallographic parameters is essential to a quantitative understanding of microstructural evolution. In an effort to extract the grain boundary energies and mobilities based on their crystallographic types, the technique for image processing and curve fitting were developed and applied to a columnar microstructure in a thin aluminum foil. The strong texture limited the boundaries observed to be predominantly low-angle boundaries. Relative grain boundary energies and mobilities have been extracted from a large set of triple junctions and mapped as a function of their crystallographic character. Boundaries based on 110 rotation axes have higher energies and lower mobilities than [111] boundaries, for example. Annealing of the foil to develop a columnar structure reveals a pronounced strengthening of the cube texture component, [001][100]. Tracking the texture at short annealing times as a mixture of cube and random orientations, simulation of grain growth using the Monte Carlo model and the experimentally derived boundary properties reveals a similar strengthening of the cube component at the expense of the randomly oriented grains. No abnormal grain growth occurs in this case. This work was supported primarily by the MRSEC Program of the National Science Foundation under Award Number DMR-0082956.
11:15 AM Y1.7
GRAIN GROWTH IN THE SYSTEMS WITH ANISOTROPIC GRAIN BOUNDARY ENERGY AND MOBILITY: THEORETICAL MODEL AND COMPUTER SIMULATION. A. Kazaryan, Y. Wang, S.A. Dregin and Bruce R. Patton, Ohio State Univ., Columbus, OH.

Grain growth in systems with anisotropic grain boundary properties is investigated by means of both computer simulation and analytical approach. Energy and mobility of the grain boundaries are considered to be anisotropic with respect to both inclination and orientation of the boundaries. It is shown that mobility anisotropy alone does not significantly change the growth kinetics of the system, even though grain shapes evolve in a non-self-similar fashion. It is the energy anisotropy that is responsible for dramatic changes in the grain growth kinetics of an anisotropic system as compared to the isotropic case. A variety of topological and morphological features are investigated and analyzed. Possible applications of the model to the problems that require anisotropic boundary properties will be discussed.

11:30 AM Y1.8
THREE DIMENSIONAL GRAIN GROWTH SIMULATIONS. M.C. Doremus, A.P. Kuprash, N.N. Carbon, D.C. George, G.K. Straub, A.D. Rollett, Carnegie Mellon University, Department of Materials Science and Engineering, Pittsburgh, PA. 1Theoretical Division, Los Alamos National Laboratory, NM. 2Computational Materials Group, Digital DNA Laboratories, Motorola, NM.

Three dimensional grain growth simulations were performed by the gradient-weighted moving finite element method [1]. Interface motion is assumed to obey a linear equation (v = m - k), where m is reduced mobility, v is the velocity, and k is the curvature of the grain boundary. An important result of the model is that the expected power law dependence of growth kinetics is obtained [2]. The gradient in mobility has a major effect on the growth process and the growth is isotropic without orientation dependence. The orientation dependence of the boundary mobility is introduced in order to break this symmetry [3]. Additionally, experimental results on grain boundary properties and grain growth that are obtained from Orientation Imaging Microscopy are compared with the simulation results.

References:

11:45 AM Y1.9
PHASE FIELD MODEL OF CRYSTAL GRAINS. Alexander E. Lobbekovs, James A. Warren, National Institute of Standards and Technology, Gaithersburg, MD.

We analyze a two-dimensional phase field model designed to describe the dynamics of crystalline grains. The phenomenological free energy is a function of a complex order parameter whose amplitude reflects the orientational order. Its phase is the predominant local orientation of the crystal. We consider the gradient flow of this free energy. Solutions can be interpreted as ensembles of grains (in which the phase of the order parameter is approximately constant in space) separated by grain boundaries. We study the dynamics of the boundaries as well as the rotation of the grains. In the limit of the infinitely sharp interface, the normal velocity of the boundary is proportional to its curvature and its energy. We obtain explicit formulas for the interfacial energy and mobility and study their behavior in the limit of a small miscorrelation. We calculate the rate of rotation of a grain on the sharp interface limit and find that it depends sensitively on the choice of the model.

SESSION Y2: INTERFACE MOTION II - MICROMECHANICS
Chair: Anthony D. Rollett and Mark Alexander
Monday Afternoon, November 27, 2000
Independence E (Sheraton)

1:30 PM Y2.3
THE INFLUENCE OF GRAIN JUNCTION DEFECTS ON GRAIN GROWTH. Alex King, Purdue University, School of Materials Engineering, West Lafayette, IN.

The structure and behavior of grain boundaries have been studied for more than a century, but little attention has been given, yet, to other grain junctions such as triple lines and quadruple points. In this presentation, we consider the possible defect contents of these line and point junctions and how they affect their motion during grain growth. We provide a simple picture of triple junction drag, which may cause grain growth stagnation. We also discuss the energetic contributions of triple junctions to the driving force for grain growth, and consider how inductive or repulsive interactions between the junctions can affect the process of grain growth. The latter two effects are shown to be particularly important in nanocrystalline materials.

Acknowledgement
This work is supported by the National Science Foundation, grant number DMR 0096147.

2:00 PM Y2.2
ATOMIC-LEVEL MODELS OF TRIPLE JUNCTIONS AND THE ORIGIN OF TOPOLOGICAL CHANGES IN MICROSTRUCTURAL EVOLUTION. Alessandro Stachowiak and Luciano Colombo, Istituto di Fisica, Universita di Cagliari, Cagliari, ITALY; Fabrizio Ceri, ENEA, Divisione Materiali, Centro Ricerche Casaccia, and INFN, Roma, ITALY.

Triple junctions are crucial elements in microstructural evolution: for example, their mobility can be rate-limiting if lower than that of grain boundaries. However, very little is known about their atomic-level structure and properties. We studied the atomic structure of multiple-twinned triple junctions in silicon, formed by the convergence of two [111] and one [221] symmetric tilt grain boundaries. Molecular dynamics simulations with the Stillinger-Weber potential and constant stress at the triple junction configurations, obtained by different combinations of the three grain boundaries. All the configurations have a positive excess line energy, a measurable volume contraction and display regions of opposite, tensile and compressive residual stress. We propose that triple junctions comprising twin boundaries could have the largest possible values of line tension and residual stress and discuss the elastic stability of polycrystalline Si. Moreover, we tried to elucidate the role of triple junctions as seeds of the first cracks: microscopic events that can lead to topological changes in the microstructure. Such events, usually dubbed as T1 and T2 in mesoscopic models in two dimensions, correspond to grain splitting (in the Ashby-Verral sense) and grain disappearance events, respectively. We present preliminary results of the atomistic modeling of both classes of topological events and discuss the connection between atomic and mesoscopic modeling of microstructural evolution. Work funded in part by the INFN-Forum Project MUSIC "Multiscale Simulation of Complex Materials"; FC also acknowledges funding by the ENEA Project FOTO "Laser-induced recrystallization of amorphous silicon".

2:15 PM Y2.3
ROLE OF GRAIN ROTATION IN GRAIN GROWTH BY MOLECULAR-DYNAMICS SIMULATION. A.J. Hasel, S.R. Phillips, D. Wolf and D. Maloyan, Materials Science Division, Argonne National Laboratory, Argonne, IL.

We have carried out molecular-dynamics simulations to elucidate the mechanism of grain growth in a thin film of nanocrystalline palladium with columnar grain structure. The conventional point of grain growth is the process governed by curvature-driven grain-boundary (GB) migration. However, in our simulations grain rotation, leading to the coalescence of grain boundaries, plays an equally important role in grain growth. In fact, our simulations reveal that the early stages of grain growth are dominated by such rotation-coalescence events, which form highly elongated grains.

Detailed analysis shows an intricate coupling between this mechanism and the conventional GB-migration driven mechanism. Incorporation of these insights into mesoscopic models enables more realistic mesoscopic simulations of grain growth.

#Work supported by the U.S. Department of Energy, Office of Science, under Contract W-31-109-Eng-38.

2:30 PM Y2.4
HREM INVESTIGATION OF GRAIN BOUNDARY MIGRATION MECHANISMS. K.L. Merkle and L.J. Thompson, Materials Science Division, Argonne National Laboratory, Argonne, IL; F. Philipp, Max-Planck-Institut für Metallforschung, GERMANY.

High-resolution transmission electron microscopy (HREM) was used to study atomic-scale grain boundary (GB) migration in grain-boundary-engineered Au thin films prepared by a special epitaxy process [1]. Twist and general GBs in addition to [110] and [101] tilt GBs could thus be prepared for HREM observation. Hence, for the first time it was possible to observe the atomistic-scale motion of high-angle twist and GBs with finite twist and tilt components. Migration of GBs can proceed in thermal activation and in the presence of point defects created by the high-energy electron beam. In the absence of a driving force one expects positional fluctuations of the
GB. The degree to which these fluctuations manifest themselves under observation in the HREM depend on the mechanism. The latter could involve point defects, vacancy motion, dislocation climb, or collective rearrangements of groups of atoms and would be dependent on the GB geometry. We will demonstrate a variety of migration modes at different facets of a bicrystal near angle ≈ 9, where the different GB inclinations strongly affect GB mobility. The most striking observation involves collective effects, where a small group of atoms transforms back and forth between two neighboring grains. The transformation is virtually instantaneous within the time resolution of the experimental setup whenever the residence time is typically orders of magnitude longer. Such fluctuations have also been observed at the core of a triple junction. The difference in surface energy between the (110) and (100) grains provides a driving force for migration of twin and general GBs and the GB typically moves by the propagation of atomistic-scale steps. The analysis of HREM video sequences indicates that migration mechanisms of high-angle general GBs may also include cooperative effects, whereby small groups of atoms spontaneously rearrange their lattice positions to be incorporated into the growing grain. These observations have shed considerable light on atomistic GB migration mechanisms and are consistent with theoretical considerations and molecular dynamics modeling studies of grain boundary migration in the literature. [1] K. L. Meckle and L. J. Thompson, Phys. Rev. Lett. 83, 556 (1999). This work was supported by the U. S. Department of Energy under contract No. W-31-109-ENG-38.

To be presented at the MRS meeting Boston, MA, November 27- December 1, 2000

SESSION Y3: INTERFACE ANISOTROPY

Chair: Anthony D. Rollett and Mark Asadov

Monday Afternoon, November 27, 2000

Independence E (Sheraton)

3:30 PM *Y3.1

ANISOTROPIC GRAIN BOUNDARY PROPERTIES FROM ATOMICISTIC CALCULATIONS

David J. Srolovitz, Moncef Ummarzu, Mikhail Mendelev, Princeton Univ, Princeton Materials Institute, Princeton, NJ.

In most models of grain growth phenomena, grain boundary properties are assumed to be isotropic. On the other hand, grain boundary mobility can vary by several orders of magnitude and grain boundary energy by a factor of two (not including low angle boundaries) from boundary-to-boundary. Part of this variation can be attributed to variation in grain boundary structure and part to grain boundary segregation phenomena. In this presentation, we examine both the intrinsic and extrinsic factors that affect grain boundary mobility, energy, morphology, and migration mechanisms. First, we present recent molecular dynamics simulation results on boundary mobility as a function of microstructure and temperature. The resulting activation energies for boundary migration are significantly smaller than those measured in high purity metals. The discrepancy is likely associated with boundary segregation effects - even in the purest metals. In order to understand the effects of segregation and its effect on the anisotropy of boundary migration, we performed a series of kinetic Monte Carlo simulations of boundary migration in the presence of diffusing impurities. Comparison of these results with available experimental data show very good agreement. The present results also clarify shortcomings in the existing theories of grain boundary migration.

4:00 PM *Y3.2

GRAIN BOUNDARY DEFACETING: A FIRST ORDER PHASE TRANSITION BY ATOMIC SHUFFLE

J.C. Hamilken, Ivan Danil, Sandia National Laboratories, Livermore, CA.

The motion of grain boundaries plays a critical role in determining the properties of thin films. A classic experiment by Heisch and Balluffi shows a reversible defaceting transition of coherent twin boundaries in an aluminum thin film at about 400 K. We initially modeled this transition using molecular dynamics and learned that the grain boundaries could move only by a cooperative motion of four atoms at the grain boundary junction. Such an excitation transforms one primitive cell of the coincidence site lattice from one grain orientation to the other thereby moving a portion of the grain boundary. This elementary excitation was mapped onto a simple trans-dimensional lattice model incorporating both the topology of the boundary and the dynamics associated with the excitation of a Metropolis Monte Carlo algorithm that we showed the defaceting transition is in fact a first order phase transition. The lattice model described here is applicable to studies of grain coarsening, and grain mobility in other thin film systems. [TE Heisch and R.W. Balluffi, Observations of Roughening/Defaceting Phase Transitions in Grain Boundaries, Acta metall. Vol. 37, 2123 (1989).]

4:30 PM *Y3.3

A NEW CONTINUUM SCALAR MODEL OF FACETS. Tinghui Xin, Huaping Wang, Louisiana State Univ, Dept of Mechanical Engineering, Baton Rouge, LA.

Facet formation and evolution are important in many processes, such as crystal growth, solidification, and grain growth during annealing. Current models of facets usually choose a particular form of anisotropic surface energy and then compute the interface profile. This approach works fine if the surface energy anisotropy is weak and the interfacial profile is relatively smooth. However, when the anisotropy increases, the surface profile starts to intersect itself. This non-uniqueness makes it difficult to model strong anisotropy in interfacial evolution. We have developed a new scalar model of facets that eliminates the non-uniqueness of interfacial profile. Planar facets and sharp corners can be easily handled by the new model. In addition, it can be incorporated directly into different theories of interfacial evolution. The new model also allows a simple proof of Wulff's theorem. In this talk, we will present the new model and discuss its applications.

4:45 PM *Y3.4

MORPHOLOGICAL EVOLUTION OF FULLY FACETED GRAIN BOUNDARIES. D.L. Medlin, G.A. Lucatino, Thin Film and Interface Science Department, Sandia National Laboratories, Livermore, CA.

Understanding the mechanisms of interface motion is critical to successfully predicting and controlling the development of microstructure. Of increasing interest are grain boundaries possessing strongly anisotropic properties which, in some systems, lead to a fully faceted microstructure. To provide a better understanding of the factors controlling the evolution of such systems, and in particular, to identify the role of the joint facets, we are investigating interfacial dynamics in the FCC Si3 system [111] oriented Au films consisting of two 180 degree related orientation variants have been produced through epitaxial deposition. The boundaries between these two variants are characterized on the microscopic level by fine scale [112] facet steps. In situ transmission electron microscopy observations allow us to study the interfacial dynamics in this system at elevated temperature. Detailed analysis of the boundary motion points to the importance of facet junction nucleation and annihilation processes in controlling the morphological evolution. This work is supported by the U.S. Department of Energy under contract No. DE-AC04-94AL85000 in part by the Office of Basic Energy Science, Division of Materials Science.

SESSION Y4: INTERACTION OF PHASE AND DEFECT MICROSTRUCTURES

Chair: Michael Zaiser and Michael V. Gluzov

Tuesday Morning, November 28, 2000

Independence E (Sheraton)

8:30 AM *Y4.1

PHASE FIELD MICROEFFECTIVITY APPROACH IN MODELING MICROSTRUCTURE EVOLUTION. A.G. Khachaturyan, Y.M. Jin, Rutgers Univ, Department of Ceramic and Materials Engineering, Piscataway, NJ; Y.U. Wang, Rutgers Univ, Dept of Mechanical and Aerospace Engineering, Piscataway, NJ. A. Artemey, Carleton Univ, Dept of Mechanical and Aerospace Engineering, Ottawa, Canada.

Because of its long-range nature, the elastic strain generated by the coherent phase transformation of different types and by lattice defects plays a major role in the mesoscopic microstructure evolution. The effect of the elastic strain is well described by the Phase Field Micromechanics theory proposed by one of the authors years ago. Being incorporated in the Phase Field formalism, the Phase Field Micromechanics theory provides the computational model, which makes it possible to realistically simulate 3-dimensional simulations of mesoscopic microstructures in coherent multiaxial and multidomain systems during decomposition, ordering and martensitic transformation in single crystals and polycrystals (with and without crystal lattice defect). This approach is naturally extended to describe domain structures in ferromagnets and ferroelectrics. Further extension of the model has allowed us to relate the physical properties of systems (mesoscopic strain, magnetization, polarization) to structural changes caused by applied external fields (stress, magnetic field, electric field). Using the Phase Field Micromechanics theory, we also have been able to formulate a new Phase Field model of dislocations that describes an evolution of an arbitrary ensemble of individual dislocations under applied stress. The model is finally taken into account the strain-induced longrange interaction dislocations and other defects, their generation and annihilation. This model can be a basis for a new approach 3-dimensional simulations of plastic deformation on the mesoscopic level as well as for...
characterization of the effects of plastic deformation on the mesoscopic microstructure formed during phase transformations.

9:00 AM Y4.2
A PHASE FIELD MODEL FOR INTERACTING DEFECT AND PHASE MICROSTRUCTURES. S.Y. Hu, L.Q. Chen. Penn State University, Department of Materials Science & Engineering, University Park, PA.

A diffuse-interface field model is proposed for describing diffusion processes in coherent systems with arbitrary microstructures and arbitrary spatial distribution of structural defects like grain boundaries, internal dislocations, grain boundaries, cracks, and inclusions. It takes into account the effect of both the coherence elastic energy of a microstructure and the elastic coupling between the coherency strains and defect strains. In this model, any arbitrary spatial distribution of defects is described using the micromechanics concept of space-dependent dislocation density tensors and the “stress-free” or “eigen” strains. Specifically, the solute segregation as well as the nucleation and diffusional growth of a coherent precipitate around an edge dislocation, dislocation glide bands, and crack-like defects are considered. It is shown that coherent precipitation may become barrierless under the influence of the local elastic field of structural defects.

9:30 AM Y4.3
MICROSTRUCTURAL DEVELOPMENT UNDER NON-ISOTHERMAL CONDITIONS. W.M. Wriggers, W. Herrmann, University of Karlsruhe, Karlsruhe, Germany.

Processings constraints on superalloys generally require that non-isothermal cooling and heating be used somewhere in the processing history. The Phase Field method, because of its ability to handle realistic volume fractions and to account for elastic interactions between phases, shows promise in these systems. However, non-isothermal transformations have thus far been the most common applications of the Phase Field method, partly because non-isothermal processes require treatment of concurrent nucleation and growth. The authors have previously proposed a method whereby nucleation and growth occur simultaneously in developing microstructures via explicit nucleation events and have demonstrated the method under isothermal conditions. This work extends the previous work to non-isothermal conditions and uses continuous cooling. Results of non-isothermal processing on transformation behavior and microstructural evolution will be given.

9:45 AM Y4.4
PHASE FIELD MICROELASTICITY MODEL IN STUDY OF THE INFLUENCES OF DEFECTS ON MARTENSITIC MICROSTRUCTURE EVOLUTION. Yongmei M. Jin, Rutgers University, Dept. of Chemistry and Materials Engineering, Piscataway, NJ; Andrew Artemeyev, Carleton University, Dept. of Mechanical and Aerospace Engineering, Ottawa, Canada; Armen G. Khachaturyan, Rutgers University, Dept. of Ceramics and Materials Engineering, Piscatawy, NJ.

The Phase Field Microrheology (PFM) theory of the martensitic transformation is extended to study the transformation in polycrystals. The theory is used to formulate the 3-dimensional model of the martensitic transformation in polycrystals and single crystals with defects. The model does not impose any prior constraints on geometry of microstructure and the structural changes during microstructure evolution. The effect of grain boundaries and defects on morphology, thermodynamics, and dynamics of the martensitic transformation is investigated. This includes study of defect-induced heterogeneous nucleation and the influences of various defects, such as precipitates, dislocations, and grain boundaries, on the development of the martensitic morphology under various temperature and applied stress. Examples of 3D simulation are discussed. The specific case of the shape memory NITI alloy is considered.

10:30 AM Y4.5
FROM THE ELECTRONIC STRUCTURE TO THE MICROSCOPIC BEHAVIOUR: A MULTI-SCALE ANALYSIS OF PLASTICITY IN INTERMETALLIC COMPOUNDS. Manfred Fähnle, Susanne Kohlhammer, Gabriel Bester, Max-Planck-Institut für Metallforschung, Stuttgart, Germany; G. Schoeck, Institut für Materialphysik, Universität Wien, Austria.

Various intermetallic compounds are candidates for high-temperature applications. Thereby some materials exhibit a non-monotonic temperature dependence of the critical yield stress with a desired maximum at high temperatures [e.g. Ni3Al] whereas others show a monotonic decrease with increasing temperature [e.g. PtAl and doped Al15], although they crystallize in the same structure as Ni3Al. It is demonstrated by a multiscale analysis that these differences can be traced back to differences in the electronic structure. A structural model for the non-monotonic yield stress, the Koop-Leckner model, which relates the microscopic plastic behaviour to the structure of the individual superdislocations. The atomic structure of the dissociated superdislocations is determined by the generalized Peierls model which is a combination of micro-elasticity theory and discrete lattice theory. The atomistic input information required for this model is provided by the ab-initio density functional electronic theory. It is shown that these differences in the electronic bonding properties (e.g. different types of hybridization between atom-localized orbitals) for different materials are reflected in different properties of the generalized stacking fault energies, and that the resulting differences in the atomistic structure of the superdislocations obtained by the generalized Peierls model are consistent with the different temperature behaviour of the critical yield stress.

Finally, it is shown how atomistic parameters for the mesoscopic modeling of dislocation processes by computer simulations may be obtained by a combination of ab-initio electron theory with the generalized Peierls model. As an example, the recombination energy of bow-tie dislocations which controls the type of cross-slip between the crystallographic planes and hence the rate of dislocation self-trapping is calculated for Ni3Al.

11:00 AM Y4.6
AMPLITUDE EQUATION FOR DYNAMIC STRAIN AGING: BEYOND LINEAR STABILITY ANALYSIS OF SERRATED FLOW IN METALLIC ALLOYS. S.N. Rashleigh, Physics Dept., Vanderbilt University, Nashville, TN; M.V. Glenzer, F. Boch, D.J. Lege, Alcoa Technical Center, Alcoa Center, PA.

The McCormick model for dynamic strain aging is explored using modern methods of nonlinear dynamics. The quasiperiodic (five-period) Ginzburg-Landau (GL) amplitude equation for the hard-mode instability is derived in the weakly nonlinear regime using the standard perturbative techniques. The goal of the present work was to go beyond the linear stability analysis to probe the parameter space area to identify those strain rate - temperature - machine stiffness parameter ranges, which correspond to different regimes of serrated flow. It is demonstrated that the amplitude equation is universal, and its bifurcational behavior in different regions of the parameter space parameter space can be either subcritical or supercritical. For the subcritical bifurcation there exists a stable limit cycle near the bifurcation threshold, while for the supercritical bifurcation the “radius” of the limit cycle depends on the control parameter. This implies that stress serrations of well-defined frequency and amplitude may develop. The analysis of the GL equation yields the bifurcation diagram which is in very good agreement with the diagram obtained numerically, i.e., the amplitude equation is accurate enough in the weakly nonlinear regime. The mathematical technique developed here was applied to a specific 6xx series aluminum alloy and yielded promising results in terms of predicting the Luder’s and PLC-free regions in the “strain rate - temperature - machine stiffness” parameter space.

11:15 AM Y4.7
EFFECTS OF DISLOCATION RELAXATION ON PHASE TRANSFORMATIONS IN SOLIDS. Alexander L. Roybard, Department of Materials and Nuclear Engineering, University of Maryland, College Park, MD.

The effect of the relaxation on microstructure, thermodynamics and kinetics of deformationless transformations is considered. Internal stresses in a transforming crystal stimulate formation and movement of defects, especially dislocations, in the vicinity of interfaces as a result of plastic deformation occurring in a new phase during its formation. The elastic fields of these interface dislocations compensate the fields of coherent segments of the interface. Therefore, partial conversion of the elastic energy into interfacial energy takes place. This effect can dramatically change the energy barrier for nucleation. On the other hand, the interface dislocations at great extent define the mobility of interface. Depending on degree of the plastic relaxation the spectrum of kinetic types of the transformation can exist.

11:30 AM Y4.8
SCREENING AND STOCHASTICS IN MICROSTRUCTURE EVOLUTION. M.E. Glicksman, Ke-Gang Wang, MS&E Department, Reinhardts Polytechnic Institute, Troy, NY; S.P. Mesh, Physical Metallurgy Branch, Naval Research Laboratory, Washington, DC.

Phase coarsening plays a fundamental role in late stages of microstructure evolution. Numerous processes, such as creating, intersecting, and joining of crystals, and their inter-diffusion depend on phase coarsening. A continuum theory of phase coarsening employing global constraints was developed several years ago on the basis of LimitAtom diffusion and screening to account for the effect of finite volume fraction on coarsening. Despite the increasing sophistication of such deterministic approaches, theoretical predictions persist in yielding unrealistically narrow particle size
distributions (PSD's) when compared to those observed in careful experiments and simulations. Recently, for example, this approach was extended using a mean-field formulation similar to that proposed by Morkoç and Ross. Their approach accounts for multiparticle interactions approximated through Debye screening. In addition, we have begun to include fluctuations of individual particle growth rates arising from variations in the local microstructural environment, or locale. Our initial estimates of the PSD and the theoretical coarsening rates agree well with recent simulations. The physical and mathematical foundations for this type of stochastic approach will be outlined. Our previous simulations of microstructure evolution in large clusters also provide insight into the nature of microstructural fluctuations in dilute systems. These fluctuations arise from stochastic variations of the locale surrounding every particle, i.e., each particle is embedded in a unique space consisting of different sized neighbors placed at different locations. Microstructural locales are included through formulation of the coarsening kinetics as a Fokker-Planck equation. The inclusion of these locale not only broaden the PSD and eliminate the need for the well-known LWJ stability criterion based on mass conservation. Progress in applying stochastic and diffusion screening in coarse-grained microstructure and microevolution theory will be discussed.

11:45 AM Y4.9
PHASE FIELD METHODS AND DISLOCATIONS A. Fine, Lab d’Etude des Microstructures (ONERA-CNRS), Cédex, FRANCE; D. Rodney, IEM (ONERA-CNRS), Cédex, FRANCE.

We present a general formalism for incorporating dislocations into Phase Field methods. This approach is valid for any 3-dimensional anisotropic elastic media with any dislocation distribution. The method is illustrated through the simulation of the dynamics of a phase separating system in presence of static dislocations. Finally, it is also shown how to incorporate the dynamic equations of the dislocations into the same formalism. This extends the applicability of the Phase Field methods to the new area of plastic properties of crystalline solids.

SESSION V: SOLIDIFICATION
Chairs: Mark D. Astar and Anthony D. Rollett
Tuesday Afternoon, November 28, 2010
Independence E (Sherron)

1:30 PM Y5.1
BRIDGING LENGTH SCALES IN SOLIDIFICATION BY LINKING ATOMIC AND PHASE-FIELD SIMULATIONS. Joe Bragaard, Askin Karma, Physics Dept., Northeastern Univ., Boston, MA; Marius Prigge, Laboratoire de Physique de la Matière Condensée, CNRS/Ecole Polytechnique, Palaiseau, FRANCE.

A Computational Materials Science Network (CMSN) was recently created that brings together atomic and continuum scale simulations in order to significantly enhance the predictive capabilities of the most computational models of microstructural evolution. This talk will focus on the solidification part of this effort and will discuss more specifically how results of molecular dynamics simulations (discussed in another presentation in this symposium) can be used as inputs to the more computationally intensive models of microstructural evolution.

2:00 PM Y5.2
A METHOD FOR OBTAINING THE ANISOTROPY OF THE SOLID-LIQUID INTERFACIAL FREE ENERGY FROM ATOMIC SIMULATIONS J.J. Hoyt, Sandia National Laboratories, Livermore, CA; M. Astar, Dept. of MSE, Northwestern University, Evanston, IL; A. Karma, Physics Dept., Northeastern University, Boston, MA.

The microporosicle solvility theory of solidification predicts that the growth rate of a dendrite is very sensitive to the small anisotropy of the solid-liquid interfacial free energy. Despite its importance in the modeling of solidification morphologies, however, very few studies have successfully measured or computed the anisotropy. We present a method of extracting the small anisotropy by monitoring the fluctuations of a crystal-melt interface during molecular dynamics simulations. When applied to the case of pure Ni modeled using embedded atom potentials, an average value of 326 mJ/m² is found for the interfacial energy, in good agreement with empirical estimates, and an anisotropy of the order of 10⁻³ is obtained. In addition, by computing the appropriate time correlation function of the interface fluctuations, the kinetic coefficient µ can be obtained. The results are in good agreement with previous computations of the interface kinetics for Ni and yield values of µ = 4.5, 32 and 18 cm/s/K for the 100, 110 and 111 directions respectively. This work is supported by the Department of Energy under contract number DE-AC04-94AL85000.

2:30 PM Y5.3
DETERMINING THE ANISOTROPIC FREE ENERGY AND MOBILITY OF LIQUID-SOLID INTERFACES FROM MOLECULAR DYNAMICS SIMULATIONS. James R. Morris, Zhong-Yi Li, Y.Y. Ye and K.M. Ho, Iowa State University, Ames Laboratory, U.S. DOE, and Department of Physics and Astronomy, Ames, IA.

The anisotropy of the liquid-solid interfacial free energy and mobility is a key parameter for studying the directional solidification, despite its small value (estimated on the order of 1% in metals). We are currently testing approaches for calculating the interfacial stiffness of interfaces, which is directly related to the free energy but exhibits a significantly larger anisotropy. We have carried out long molecular dynamics simulations of liquid-solid interfaces in aluminum using an embedded atom potential. Through calculations of the height-height correlation function of the fluctuating interface, we can obtain accurate interfacial stiffnesses along different directions. We also examine new approaches for calculating the mobility, by examining the dynamics of the interface as a function of time.

2:45 PM Y5.4
ATOMIC-SCALE COMPUTER SIMULATIONS OF SOLIDLIQUID INTERFACES IN Co-Ni ALLOYS. Harish Ramasimhan and Mark Astar, Northwestern University, Dept. of MSE, Evanston, IL; J.J. Hoyt, Sandia National Laboratories, Livermore, CA.

The thermodynamic and kinetic properties of solid-liquid interfaces are of paramount importance in the modeling of solidification. We focus on the Co-Ni alloy system, modeling the properties of solid-liquid interfaces using atomistic simulation techniques. We establish a stable equilibrium interface using Monte-Carlo simulation, and study variation in composition, density and energy normal to the interface. From these results we account for equilibrium solidification and liquidus boundaries predicted by the embedded atom method and interatomic potentials used in our simulations. The equilibrium structures obtained from Monte-Carlo provide the starting point for molecular-dynamics simulation studies of the equilibrium dynamical properties of solid-liquid interfaces in Co-Ni alloys. This work is supported by the Department of Energy under contract number DE-AC04-94AL85000.

3:30 PM Y5.5

Microgravity dendritic growth experiments, conducted aboard the space shuttle Columbia (STS-47) in November/December 1997, are analyzed and discussed. In situ video images new reveal that pivalic acid (PVA) dendrites growing in the diffusion-controlled environment of low-earth orbit exhibit a range of growth behaviors, including steady, transient, and oscillatory states. The observed frequency of the growth process are being studied with the objective of understanding the physical mechanisms responsible for these behaviors. Transients in the observed growth speed are thought to arise from an intrinsic aspect of the evolving dendritic pattern. Variability in the growth speed observed from a sequence of otherwise identical runs at equal supercooling suggests that self-interactions of the dendrite remain important throughout the development of the dendritic pattern. A Green function analysis of the near-tip diffusion sources contributing to the local field at the tip suggests that strong non-local interactions exist well into the time-dependent side-branch region of real dendrites. Video data obtained at 30 fps allow the first application of discrete Fourier transform methods (Lomb- periodograms) to the digitized images of dendritic growth under quiescent microgravity conditions. These observations provide evidence for the appearance of characteristic frequencies in the tip shape and its dynamical behavior. Some of the frequency bands observed coincide closely with the ratio of the dendritic tip growth speed divided by the side branch spacing. Other observed lower frequencies remain as yet unexplained. These data might be interpreted on the basis of a limit cycle operating near the tip of the dendrites. These data, and their interpretations, will be discussed.

4:00 PM Y5.6
SIMULATION OF THE RHEOLOGY OF A THIXOTROPIC ALUMINUM ALLOY BY USING A TWO-PHASE FLOW APPROACH. A. Ludwig, M. Wu, RWTH Aachen, Rheinisch Westfälische Technische Hochschule, Aachen, GERMANY.

Semisolid metal alloys exhibit a shear-rate history-dependent flow
response during injection into a die. The increasing interest from the thin-sheet industry makes the understanding of the flow behavior of the thixotropic alloys necessary. The liquid material is frequently measured with a capillary viscometer. This technique was used to investigate the rheology of semisolid alloys by applying a two-phase flow approach. The model considers both the liquid and the solid phases to behave as separate fluids with their own viscosities. The interaction between the wall adhesion, the different viscosities of the solid and liquid phases and the momentum exchange between the phases determine the phase separation within the capillary tube and the apparent viscosity of the mixture. The effect of different "solid-viscosity" formulations and different momentum exchange models on the flow process within the capillary viscometer is studied and discussed.

4:15 PM *Y5.7
DISLOCATION STRUCTURE OF ALUMINUM ALLOYS AFTER NONEQUILIBRIUM CASTING.* Vidam S. Zlotowski, Moscow Institute of Steel & Alloys, Department of Physical Metallurgy of Nonferrous Metals, Moscow, RUSSIA.

The dependence of the dislocation structure of cast aluminum alloys on composition and rate of cooling (VC) during solidification was systematically investigated. The main method of structure analysis was transmission electron microscopy. Experiments were carried out with polycrystalline binary (Al with Cu, Mg, Si, Zn, Mn, Ge, Be) and multicomponent alloys of the systems Al-Cu-Mg, Al-Zn-Mg, and Al-Si-Mg-Cu. In the equilibrium condition all alloys possessed a single phase structure of aluminum solid solution (Al). VC was varied in the interval 10\(^{-5}\) - 10\(^{-2}\) K/s. It was determined that at VC\(<\)20 K/s (Al most of the grain boundaries along the cellular interlamellar structure, and at VC\(\geq\)8.14 K/s, a polygonal (subgrain) type structure forms, whereas in the alloys with lesser Mg content and in the ternary Al-Zn-Mg alloys a mixed (cellular + subgrain) type of structure forms. The total dislocation density in all the alloys usually falls within the m range of one order of magnitude: 10\(^{-2}\) - 10\(^{-6}\) cm\(^{-2}\) sometimes \(<10^6\) (at small VC) or 10\(^{10}\) - 10\(^{15}\) cm\(^{-2}\) (at maximum VC and subgrain structure). The difference between dislocation densities in the cast alloys has a significant influence on the tensile yield strength. The subgrain size in the Al-Mg alloys with polygonal structure is directly proportional to the dendrite cell size. Parameters of dislocation structure in different microvolumes inside a dendrite cell are related to the concentration profiles of alloying elements. The solutions with Mg contents of 0.1\% have a density of one order of magnitude: 10\(^{-2}\) - 10\(^{-6}\) cm\(^{-2}\) sometimes \(<10^6\) (at small VC) or 10\(^{10}\) - 10\(^{15}\) cm\(^{-2}\) (at maximum VC and subgrain structure). The difference between dislocation densities in the cast alloys has a significant influence on the tensile yield strength. The subgrain size in the Al-Mg alloys with polygonal structure is directly proportional to the dendrite cell size. Parameters of dislocation structure in different microvolumes inside a dendrite cell are related to the concentration profiles of alloying elements. The solutions with Mg contents of 0.1\% have a density of one order of magnitude: 10\(^{-2}\) - 10\(^{-6}\) cm\(^{-2}\) sometimes \(<10^6\) (at small VC) or 10\(^{10}\) - 10\(^{15}\) cm\(^{-2}\) (at maximum VC and subgrain structure). The difference between dislocation densities in the cast alloys has a significant influence on the tensile yield strength. The subgrain size in the Al-Mg alloys with polygonal structure is directly proportional to the dendrite cell size. Parameters of dislocation structure in different microvolumes inside a dendrite cell are related to the concentration profiles of alloying elements. The solutions with Mg contents of 0.1\% have a density of one order of magnitude: 10\(^{-2}\) - 10\(^{-6}\) cm\(^{-2}\) sometimes \(<10^6\) (at small VC) or 10\(^{10}\) - 10\(^{15}\) cm\(^{-2}\) (at maximum VC and subgrain structure). The difference between dislocation densities in the cast alloys has a significant influence on the tensile yield strength.

8:30 AM *Y6.1/25.1
SPATIAL DISTRIBUTIONS OF DISLOCATION STRUCTURES FROM MILLIMETERS TO NANO METERS. Darcy A. Hughes, Center for Materials and Engineering Sciences, Sandia National Laboratories, Livermore, CA.

The key element describing dislocation structures formed during cold deformation in medium to high stacking fault energy Fe alloys is a cell block. A cell block is composed of cell block boundaries (flat extended geometrically perfect interfaces) and cell boundaries (short incident dislocation boundaries, IDBs). Small lattice rotations occur across the IDBs, whereas much larger and significant lattice rotations are observed from one cell block to its neighbors. This difference is in accord with N\(_s\) differences in slip patterns between neighboring cellblocks. The spacing of both types of boundaries decreases monotonically with increasing strain while the misorientation angles across them increase with increasing strain. For example, depending on the deformation conditions and material, the size of a cell block can range from 100 \(\times\) 100 \(\times\)100 micrometers to 1 \(\times\) 10 \(\times\) 100 nanometers. Misorientation angles can range from 1 to 62.8 degrees. Thus the cell blocks accumulate a record of the slip patterns. Mapping the distribution of the cell block parameters across a grain in a polycrystal or along a deformed single crystal or bicrystal, can be used to explore the larger scale effects of grain orientation, grain boundaries, as well as the constraints arising from the deformation boundary conditions such as Fixture, sample grips, and test pieces. This is illustrated by comparisons dislocation structures that form in single crystals, bicrystals and polycrystals as a function of strain.

SESSION Y6/25. JOINT SESSION STRAIN LOCALIZATION AND DISLOCATION PATTERNING

Chairs: Michael Zaiser and Elisa C. Affaiti.

Wednesday Morning, November 29, 2000
Independence (Sheraton)

8:45 AM *Y5.8
EFFECT OF ULTRASONIC (CAVITATION) TREATMENT OF THE MELT ON THE MICROSTRUCTURE EVOLUTION DURING SOLIDIFICATION OF ALUMINUM ALLOY. Georgy Eskin, All-Union Institute of Light Alloys, Moscow, RUSSIA.

During past 30 years, All-Union Institute of Light Alloys (VILS) was involved in the fundamental research on the development and application of ultrasonic (cavitation) melt treatment during DC casting of aluminum and magnesium alloys.

These studies showed the major role of acoustic cavitation in the formation, pulsation and coagulation of fine hydrogen bubbles. Such bubbles are easily formed at the surface of nonmetallic dispersed inclusion phases which are always present in the real melt. During the ultrasonic treatment under the cavitation mode, unstable fields of cavitation bubbles are formed during the tensile phase of a sound wave. These cavitation bubbles essentially change the behavior of liquid metal stratification, electrical polarization, and solidification. Because of nonlinear pulsations induced by ultrasound, cavitation bubbles start to pulsate and subsequently either transform into macroscopic gasous bubbles or collapse with the formation of powerful local hydraulic pulses and cumulative jets. These processes result in the efficient melt degassing and the formation of numerous active solidification sites. The latter is due to the noncavitation effect and the wetting of fine nonmetallic particles in the melt.

The multiple solidification nuclei generated in melt treatment changes the evolution of structure during solidification. With respect to the intensity of cavitation process in the melt ultrasonic treatment, it is possible to form the uniformly refined, nondendritic equiaxed structure instead of the usual dendritic grains. The nondendritic grains are characterized by the absence of branching. The size of such nondendritic grain is equal to the dendritic parameter of the dendritic grains formed at the same cooling rate conditions but without ultrasonic treatment.

Our studies indicate that the formation of nondendritic structure in light alloys improves plasticity of castings and ingots without loss of strength, which allows production of large-size, crack-free ingots from commercial structural aluminum alloys. The nondendritic structure of cast light alloys improves of deformed semi-products irrespective of the hot deformation conditions and thermal histories. In addition the nondendritic structure facilitates semi-solid processing of alloys.


DE-AC04-94AL85000

9:00 AM *Y6.2/25.2
DEVELOPMENT, SCALING AND EVOLUTION OF DISLOCATION CELL SUBSTRUCTURES. Elizabeth A. Holm, Sandia National Laboratories, Albuquerque, NM; Richard A. LeSuer, Los Alamos National Laboratory, Los Alamos, NM; David A. Владимиков, Dept. of Mechanical Engineering, University College Dublin, IRELAND.

The development of a dislocation cell substructure has been observed in a wide variety of plasticly deformed metals. Both cell size and cell boundary misorientation distributions follow apparently universal scaling functions, and the average size and misorientation correlate with the total plastic strain. Analysis of random dislocation arrays shows such scaling behavior; however, there is a quantitative discrepancy between theory and experiment. Monte Carlo energy minimization simulations for dislocation array evolution indicate cell formation with cell orientations more narrowly distributed than for a random array. The effect is present in two-dimensional simulations of edge dislocations and becomes more dramatic in three-dimensional systems. The narrowing of the cell orientation distribution reflects a competition between energy favoring randomness and a Gaussian cell orientation distribution) and enthalpy (favoring minimization of cell boundary energy via small misorientations). When this competition is included in the analytical theory, the experimentally observed scaling function is produced. Furthermore, this scaling is found in a variety of systems exhibiting a competition between randomness and order. The universal misorientation distribution, along with appropriate boundary motion laws, is incorporated in a cell-like automaton model of cell substructure evolution. Cell size scaling is observed. Evolution of the cell substructure occurs by uniform recovery, with selfsimilar cell size and misorientation distributions characterized by a continuously increasing average cell size.
size and a continuously decreasing average misorientation. Abnormal cell growth, which would indicate a recrystallization nucleation event, does not occur.

9:30 AM Y6.3/Z5.3
COMPUTER SIMULATIONS OF DISLOCATION CELL STRUCTURE EVOLUTION Modelled by Mark Shkolnik, Department of Mechanical Engineering, University College Dublin, Belfield, Dublin, IRELAND; Elizabeth A. Holm, Sandia National Labs, Albuquerque, NM.
The annealing behaviour of dislocation cell structures is explored using a 3D cellular automaton model of dislocation boundary evolution. A Monte Carlo technique is used to construct the initial dislocation cell structures. These are statistically equivalent to experimentally measured deformation structures. Cell boundaries contain both geometrically necessary and redundant dislocations and are thus in an nonequilibrium state at the beginning of the simulation. As a result of climb and recombination the redundant dislocation content of the boundaries decreases during the simulation. This recovery process alters the boundary energy and mobility of the dislocation cell boundaries. CURVATURE driven cell boundary migration takes place concurrently with this recovery process and coarsens the cell structure. Two distinct regimes of behaviour are identified. These are defined critically by the rate of boundary recovery. The first is normal cell growth in which the average cell boundary misorientation decreases with time and cell size increases uniformly. In the second regime an incubation period of microstructural stagnation is followed by abnormal cell growth, in which cells with high misorientation boundaries migrate and consume all other cells. It is important to note that these cells do not grow without restrictions by taking into account the statistical properties of the dislocation cell distribution. This process strongly resembles the early stages of recrystallization. We discuss the crucial role played by redundant dislocations and report on experiments to measure their density in deformed aluminium single crystals.

9:45 AM Y6.4/Z5.4
DISLOCATION PATTERNING AND VORTEX CHANNELING IN THE XY MODEL. Robin L. Selinger and Brian B. Smith, Catholic Univ. Physics Dept., Washington, DC.
To understand how dislocations form ordered structures during the deformation of metals, we study the patterning of defects in a related but simpler system, the XY roton model with twisting boundary conditions. While highly idealized, this model provides useful insight into the basic phenomena of plasticity. Vortices in the XY model are analogous to screw dislocations, and the applied twist rate is analogous to the shear strain rate. Simulations of the model in 2-D show the spontaneous formation of vortex channels, where each channel is a narrow strip along which defects flow at high density, as in a shear band. Channels are separated by wide defect-free regions, and after initial formation the channel spacing widens gradually through a coarsening process, reaching an apparent equilibrium value which varies with temperature and strain rate. Both channel spacing and overall defect density obey scaling relations with the applied strain rate. We explain this pattern formation process as a phase separation between ordered and disordered phases of the 2-D XY system, where well behaved vortices and defects undergo a phase transition. The introduction of a crack and bond-breaking rules into the model reveals a brittle/ductile transition with temperature and strain rate. Preliminary results for the 3-D XY roton model under twisting boundary conditions also show coalescence of vortex lines/loops into shear bands. Potential applications include studies of the size effect and strain gradients in plasticity, and testing the Khain-S.Papoulis-Vitek theory of the brittle/ductile transition. This model may also describe the channeling of vortices in type II superconductors.

10:30 AM Y6.5/Z5.5
DISLOCATION PATTERNING: STOCHASTIC APPROACH TO MesoSCALE MODELLING. Peter Höner, Technische Universität Braunschweig, Institut für Metallphysik und Nukleare Festkörperphysik, Braunschweig, GERMANY.
Plastic deformation by dislocation glide is known to be associated with the spontaneous formation of mesoscopic patterns of various types, e.g. cellular dislocation structures during unidirectional deformation, and periodic persistent slip band structures during cyclic deformation. While it is recognized that dislocation patterning represents a dissipative far-from-equilibrium process, theoretical modeling of these phenomena is complicated by the long-range nature of dislocation interactions inducing collective dislocation behaviour on a mesoscopic scale. In this paper the problem is addressed using a stochastic approach with random fluctuations acting on the evolution of the dislocation ensemble. The intensity of the fluctuations is determined self-consistently from dynamic dislocation interactions and, hence, reflects correlated dislocation motion. It is shown that these fluctuations may induce dislocation patterns by stabilizing non-uniform dislocation distributions. Microstructure-based models are presented for unidirectional and cyclic plastic deformation. In the first case fractal dislocation distributions corresponding to hierarchically organized dislocation cell structures are obtained, while in the latter case a deformation into discrete dislocation pile-ups or weaves and depleted channels is found, which are associated with the formation of persistent slip bands and matrix structures. The results are compared to experimental observations in single-crystalline iron, steel and nickel. The close agreement at points is the importance of collective dislocation interactions in the self-organization of those structures.

11:00 AM Y6.6/Z5.6
STATISTICAL PROPERTIES OF DISLOCATION ASSEMBLIES. I. Groma, Eszter University Budapest, Department of General Physics, Budapest, HUNGARY.
It is well known that during the plastic deformation of single crystals the dislocation distribution does not remain homogeneous. In spite of the increasing experimental and theoretical activity on this field we are far from the understanding of these typically self-organized phenomena. A possible approach for the modeling of these pattern formation processes is to investigate the collective behavior of systems consisting of individual dislocations by computer simulation. However, because of the long range character of the dislocation interaction the direct numerical integration of the equations of motion of dislocations are very computation expensive restricting considerable the affordable dislocation number or simulation volume. The aim of the investigations presented in the paper is to overcome these restrictions by taking into account the statistical properties of the dislocation assembly. In the first part of the paper it is shown that the individual (micro-scale) and the continuum (meso-scale) approaches can be linked through the construction of a hierarchy of evolution equations of the different order dislocation distribution functions. By neglecting the dislocation-dislocation correlations a self-consistent field description is derived which can be considered as a zero order approximation. In the second half of the behavior of a system of straight parallel dislocations is investigated. It is found by numerical simulation that the internal stress \( r \) created by the dislocations has a stochastic component. In order to describe this stochastic character the form of the probability distribution function of the internal stress is determined. It is shown that the mean value of the distribution function is the self-consistent field created by the dislocation, and the distribution function decays with \( r^3 \).

11:15 AM Y6.7/Z5.7
DISLOCATION MULTIPLYING IN GERMANIUM. COMPARISON OF EXPERIMENTAL AND SIMULATION RESULTS. C. Charbonnier, T. Kruml and J-L. Martin, Ecole Polytechnique Federale, Department de Physique, Lausanne, SWITZERLAND.
About dislocation multiplication and covalent crystal and the associated yield-point, several questions remain open. A study of this phenomenon is underway on Ge single crystals oriented in single glide. Monotonic compression tests are performed together with transients (repetition of creep tests at constant stress and strain-rates \( 10^{-5} \) to \( 4.10^{-3} \)). Dislocation structures are observed in the transmission electron-microscope. The conditions of chemical polishing of the lateral faces have been defined so as to remove surface defects, the presence of which affects the height of the yield-point. The transients are performed before the upper yield-point and after the lower yield-point for comparison. At similar stresses, the corresponding deformation-rate is observed to be smaller in the former part of the stress-strain curve as compared to the latter. This corresponds to a lack of mobile dislocations at the onset of deformation. The activation parameters of dislocation mobility are determined after the lower yield-point and correspond to a lattice friction mechanism. They are used to analyze the measurements before the upper yield-point, in an attempt to obtain experimental data about mobile dislocation densities as a function of time. The values of the latter parameter will be compared with those predicted from 3D simulations of Frank Read sources in a coherent monolayer of Si performed by Mounin, Condé, Kubin (Acta Mater. 1999).

11:30 AM Y6.8/Z5.8
SIMULATION OF DISLOCATION CELL STRUCTURES. Benoît Devincre, Diego Gomez-Garcia, Ludovic P. Kubin, IEM, CNRS-ONERA, Châlillon, FRANCE.
It has been known for a long time that dislocation cells are formed at low and medium temperatures in FCC single crystals deformed into stage III, or from the onset of plastic flow in multi slip conditions. In BCC crystals cell structures are also formed in conditions of strain and temperature such that the interactions between dislocations prevail.
over the lattice friction. The objectives of dislocation dynamics simulations in this domain are to reproduce dislocation cell formation, define the basic interactions that contribute to it, and understand the stress dependence of the cell dimensions (the so-called similitude principle). Results are shown of a 3-D simulation of FCC crystals deformed in multiaxial conditions at room temperature. Dislocation cells are formed at strains of the order of 0.5%. The role of various dislocation mechanisms has been cleared out by switching them on and off one by one. This leads to the conclusion that dislocation storage and the initial steps of the formation of cell structures mainly depend on short-range forces and interactions. In contrast with what is usually thought, long-range elastic interactions do not contribute significantly to the bifurcation from uniform to non-uniform dislocation microstructures. More specifically, short-range interaction stresses favor cross-slip events that lead to storage of debris and stable dislocation configurations. The latter, together with stable dislocation loops, serve as anchoring points for the formation of dislocation cells. Once the cells are formed, a pattern of long-range stresses is established that enhances their further development. Attempts to investigate the origin of the dislocation principle are discussed with the help of a 2-D simulation that mimics in 2-D the three-dimensional mechanisms described above.

11:15 AM Y6.9/25.9
STRAIN GRADIENTS AND PATTERNING OF PLASTIC FLOW. John L. Bisson, Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA.

Localized deformation during plastic flow of crystalline metals commonly leads to microstructural patterning. One of the most widely observed patterning is the lamella microstructure associated with coarse slip. We have shown that fine secondary slip that contributes significantly to overall hardening behavior also play an important role in the nucleation and stabilization of such localized modes of deformation. These secondary slip bands can also control patterning, e.g. thickness and spacing of coarse slip bands, through the effects of slip instability. In continuum theory the crystal lattice is assumed to distort only elastically, while generally the elastic deformation itself is not compatible with a single-valued displacement field. A simple gradient (nonlocal) theory is discussed in which incompatibility only occurs in the instantaneous hardening relations. As a result, the crystal distortion calculations relevant to shear localization are preserved for rate-independent behavior. Predictions for patterning of localized deformation using this theory are promising.

SESSION Y7: DISLOCATIONS AND PLASTICITY
Chair: Michael V. Glazier and Elizabeth A. Helm
Wednesday Afternoon, November 29, 2000
Independence E (Sheraton)

1:30 PM Y7.7
PHENOomenological and Experimental Development in Quantifying Plastic Deformation. Vivek John, Alcoa Technical Center, Alcoa Center, PA.

The ability to quantify plastic flow during thermomechanical processing (i.e. ability to predict flow stress during working) has several important implications in the metals industry. Hot flow stress predictions are necessary in design and control of fabrication operations such as rolling, forging and extrusion. The evolution of mechanical properties due to the generation of line defects can also be effectively predicted, if the working hardening response is quantified as a function of thermo-mechanical histories.

The efforts at modeling the constitutive response have been based on empirical, phenomenological or physically-based approaches. Phenomenological models, backed by well-designed and controlled experiments have been the most successful means of developing constitutive relationships for practical applications. Some of the state of the art experimental and modeling techniques developed at Alcoa Technical Center will be presented.

2:00 PM Y7.2
DEPINNING TRANSITION OF DISLOCATIONS. Stefano Zapperi, INFN, Università e Le Sapienze, Roma, ITALY; Michael Zaiser, MPI, Stuttgart, GERMANY.

The theory of depinning transition of elastic manifolds in random media provides a framework for the statistical dynamics of dislocation systems at yield. We first consider the case of a single flexible dislocation gliding through a random stress field generated by a distribution of immobile screw dislocations threading through its glide plane. The immobile dislocations are arranged in a "restrictedly random" manner and provide an effective stress field whose statistical properties can be explicitly computed. We write an equation of motion for the dislocation and compute the associated depinning force, which we identify with the steady depinning force. We use the solutions of a discretized version of the equation confirm these, and allow us to explore the effect of different dislocation arrangements and to investigate the critical dynamics of the pinning-depinning transition.

2:15 PM Y7.3
A STOCHASTIC GRAIN GROWTH MODEL INCLUDING DISLOCATION PLASTICITY. Filippo Cheli and Gregorio Dincauno, ENEA, Div. Struttura Materiale, Centro Ricerche Casaccia, and INFN, Roma, ITALY.

We present a stochastic microstructure evolution model applicable to grain growth and its recent extensions, in particular relative to dislocation plasticity. The model is actually implemented by means of numerical simulations based on the velocity Monte Carlo algorithm [F. Cheli, J. Phys. A 34 (2001)]. It describes the evolution of a two-dimensional microstructure by tracking the motion of triple junctions, i.e. the vertices where three grain boundaries meet. Grain boundaries can be modeled as straight or curved segments; both the misorientation dependence of grain boundary energies and mobilities can be included. We show simple examples of normal, abnormal and oriented grain growth. The stochastic contribution is shown to be fundamental in order to give the correct time-scaling behavior of topological quantities, such as grain-size distribution and average grain size. The model is already capable of dealing with a two-phase system, to simulate both grain growth and grain dissolution in the liquid. Finally, we report preliminary results of a recent extension of this model to include crystal plasticity by two different methods: (a) a mean-field method, which requires solving a stress-strain equation within each grain, whose result in turn affects the effective values of grain-boundary energy and mobility; (b) by explicitly tracking the motion of individual twin, interacting dislocations whose density and position affects grain-boundary migration. Work funded in part by the INFN/Forum Project MUSIC "Multiscale Simulation of Complex Materials" and the ENEA Project PHOTO "Laser-induced re-crystallization of amorphous silicon".

2:30 PM Y7.4
A GENERAL MONTE CARLO APPROACH FOR MODELING 3D DISLOCATION MICROSTRUCTURES. Sriram Swaminathan and Richard LeSar, Los Alamos National Laboratory, Structure/Property Relations, Los Alamos, NM.

Even though dislocations are atomic scale defects, their interactions extend over continuum scales that are several orders of magnitude greater than the atomic scale. Consequently, the best approach to study large scale dislocation interactions is one that uses dislocations as the basic entity in the simulation. To date the most successful methods used to tackle this problem is dislocation dynamics (DD) which tracks the time evolution of the microstructure by solving the equations of motion based on the forces on dislocations. In this presentation we discuss a general Monte Carlo (MC) approach as an alternate means of modeling three dimensional dislocation microstructures. We compare the MC results with theoretical and DD results for some simple cases (single dislocation loops and Frank Read sources) and discuss the relative merits and pitfalls of DD and MC approaches. We present the results of a system consisting of a large number of dislocation loops and Frank Read sources in the presence of an externally applied stress. The complex interactions between the dislocations in the system and the evolution of the dislocation microstructure is captured by the MC method. We demonstrate how the method can be extended to study the effects of other lattice defects, such as inclusions, on the equilibrium distribution of dislocations in the system.

3:15 PM Y7.5
A LANDAU-Ginzburg APPROACH TO POLYCRYSTALLINE TEXTURE ANALYSIS. Andrew Delgert, James Sethna, Laboratory of Atomic and Solid State Physics, Cornell University; Chris Myers, Cornell Theory Center.

After plastic deformation, the properties of a polycrystalline metal become anisotropic: the response to external loading, the grain morphology, the yield strength, and the fracture toughness all depend upon the past deformation history. One source of this anisotropy is the texture, the probability distribution of grain orientations in the material. We explore the remarkable analogies between some of the engineering approaches to texture and the Landau-Ginzburg theories that physicists use to describe liquid crystals, superconductors, and superfluids. We examine whether we can describe non-equilibrium problems with a systematic theory based on a Landau-Ginzburg order parameter developed from low order symmetries of the orientation distribution function. Experiments and simulations of state-of-the-art engineering models of polycrystalline texture will be used to test this reduced-order description.
3:30 PM Y7.6
ATOMIC-SCALE SIMULATIONS OF DISLOCATION, DISLOCATION AND DISLOCATION GRAIN BOUNDARY INTERACTIONS. Jakob Schiotz, Center for Atomic-Scale Materials Physics and Department of Physics, Technical University of Denmark, Kongens Lyngby, DENMARK.

In order to understand and model the plastic behavior of materials, it is necessary to obtain a good description of the fundamental processes in deformation. We have used large scale simulations on parallel computers to study the interactions of crystal defects in metal. The main focus of our simulations has been on dislocation-dislocation interactions, and on dislocation-grain boundary interactions. Dislocation-dislocation interactions: Recent experiments involving high-speed deformation of thin metal foils have shown a very high density of dislocations, and a low density of dislocation-like defects, in deformed samples. This was interpreted as evidence of a dislocation-free deformation mechanism, active at very high strain rates [M. Kiritani et al., Philos. Mag. Lett. 79, 797]. We have used molecular dynamics simulations of single crystals in bulk and have configurations to investigate this proposal. In no cases do we find evidence of a dislocation-free deformation mechanism, but we do reproduce the high rate of vacancy production seen experimentally. We have investigated the mechanism behind the vacancy production, and find that it is caused by the elimination of short segments of edge dislocations moving on adjacent slip planes. Dislocation-grain boundary interactions: We have studied the interactions between dislocations and grain boundaries by generating dislocations near a grain boundary in a stressed bicrystal. Simulations show how the grain boundary is able to confine the plastic deformation to a single grain until sufficient stress has built up in the other grain. In the case where the dislocations are generated by a microcrack, the stress field from the crack can influence the strain field near the crack edge on the same side as the crack. This results in a strong confinement of the plastic deformation, where a large amount of dislocation activity is seen in one grain, before dislocations appear in the second grain.

3:45 PM Y7.7
DISLOCATION CORE FIELDS AND THE FORCE BETWEEN DISLOCATIONS NEAR CORE OVERLAP. Chuck Henager, Jr., Howard B. Heinrich, Jr., Rick Kurty, Pacific Northwest National Laboratory, Richmond, WA; Dick Houghton, Los Alamos National Laboratory, Los Alamos, NM.

Atomic models of edge, screw, and mixed dislocations were used to determine the properties of the dislocation core field using an embedded atom method potential for Al. The core field was characterized by a force dipole field (distant center) that falls off as 1/r^3. A nonlinear least squares fitting procedure was used to obtain the locations and ellipticities of the dipoles as a function of edge and screw components by analyzing residual atom displacements relative to the Volterra field. It was found that the origin of the dipole was coincident with a dislocation line with an edge character only at an edge point at a small enough distance from the core. The relaxation procedure was further refined by placing the dipole field and the Volterra field in the initial atom configuration and relaxing to a final configuration. In this way an improved estimate of the core field was obtained by requiring that the strength of the core field is consistent with the measured core size. The relaxation procedure was then followed by allowing only the dipole field to relax. The results of the model were consistent with the predictions of the continuum theory of elasticity, but were coincident with a dislocation characterized by a force dipole field.

4:00 PM Y7.8
CHARACTERIZATION OF DISLOCATIONS ACTIVE IN MICROVOID GROWTH. James Behl and Robert E. Rudd, Lawrence Livermore National Lab., Univ. of California, Livermore, CA.

We use atomic simulations to characterize the dislocation activity in the plastic zone surrounding a void growing under tensile loading.Millions of atom molecular dynamics simulations have been run on a system initially consisting of a periodic box filled with atoms in a single crystal silic or polycrystalline array. [1] A critical strain is applied that induces void growth, which is accompanied by dislocation generation in the volume immediately surrounding the void. We have studied the resulting dislocation systems in Fe-Al metals using the Embedded Atom Method interatomic potential models representing copper. The dislocations are naturally split into partials. During the course of the void growth, the partials form junctions which are important to the mechanical properties of the void. [2] The junctions allow the formation of a dislocation loop, which facilitates outward material transport and accommodates the growing void. We further identify the character of the most numerous dislocations and their associated glide planes. The results are in agreement with experiments and simulations on parallel computers to study the interactions of crystal defects in metal. The main focus of our simulations has been on dislocation-dislocation interactions, and on dislocation-grain boundary interactions. Dislocation-dislocation interactions: Recent experiments involving high-speed deformation of thin metal foils have shown a very high density of dislocations, and a low density of dislocation-like defects, in deformed samples. This was interpreted as evidence of a dislocation-free deformation mechanism, active at very high strain rates [M. Kiritani et al., Philos. Mag. Lett. 79, 797]. We have used molecular dynamics simulations of single crystals in bulk and have configurations to investigate this proposal. In no cases do we find evidence of a dislocation-free deformation mechanism, but we do reproduce the high rate of vacancy production seen experimentally. We have investigated the mechanism behind the vacancy production, and find that it is caused by the elimination of short segments of edge dislocations moving on adjacent slip planes. Dislocation-grain boundary interactions: We have studied the interactions between dislocations and grain boundaries by generating dislocations near a grain boundary in a stressed bicrystal. Simulations show how the grain boundary is able to confine the plastic deformation to a single grain until sufficient stress has built up in the other grain. In the case where the dislocations are generated by a microcrack, the stress field from the crack can influence the strain field near the crack edge on the same side as the crack. This results in a strong confinement of the plastic deformation, where a large amount of dislocation activity is seen in one grain, before dislocations appear in the second grain.

4:15 PM Y7.9
EFFECT OF BOUNDARY CONDITIONS IN ATOMIC SIMULATIONS OF VOID GROWTH. R.R. Setogt, Dept of Civil & Environmental Engineering, Univ of California Davis, Davis, CA; B.P. Somayajulu and M.P. Hohenemser, Sandia National Laboratories, Livermore, CA; M.J. Baken, Los Alamos National Laboratory, Los Alamos, NM.

The study of microvoid growth and coalescence using atomistic simulations provides insight into the mechanisms and relevant length scales for this damage evolution process. The roles of dislocation nucleation and propagation in microvoid growth and coalescence are readily visualized using post-processed images of the lattice. In addition, length scales reduced to void size, void spacing, and lattice (area) size are inherently incorporated into the simulations. The objective of this work is to establish a foundation for conducting atomistic simulations of damage evolution. In particular, this work explores the effect of boundary conditions on microvoid growth and coalescence using the Embedded Atom Method. The following variables are examined for lattices with finite boundaries: fixed-dislocation versus free-force boundary conditions as well as radial loading versus uniform loading along the free surfaces. These simulations are compared to results from lattices with periodic boundaries. The effect of fixed loading is examined by conducting quasi-static energy minimizations as well as full-size molecular dynamics simulations. The lattices of interest are nickel containing initial one-void and two void configurations.
Thermolysis of polymer precursors leads to amorphous ceramics, which are known to exhibit high temperature stability. The absence of a liquid phase with a low melting point results in outstanding high temperature creep resistance. The mechanical properties of such materials are severely influenced by the processing conditions which are reflected on the observed structure consisting of an amorphous matrix and open as well as closed porosity. For the characterization of the high temperature behavior, isothermal creep resistance of Si-CN amorphous ceramics, isothermal compression creep tests at temperatures up to 1550 °C and stresses up to 300 MPa were performed with compression and bending samples. The Si-CN ceramic, derived from the precursor Ceraset, exhibits pronounced primary creep and no stationary creep which is likely to be due to the amorphous state of the ceramic material. It is proposed that the free volume is reduced during the creep test leading to an increase of the viscosity. The creep rates exhibit an stress exponent of approximately one for compression as well as for bending. The influence of the microstructure on the fracture mechanics of precursor ceramics is studied by crack propagation and K-curve measurements with DCL-apparatus.

**Y8.3 EVOLUTION OF MICROSTRUCTURE AND DEFECT STRUCTURE DURING NUCLEATION AND GROWTH OF THE Li1.2 PHASE IN MANGANESE-LANTHANUM-ALUMINUM CRYSTALS**

Cagnacc Yang, Jorg M.K. Weizcek, William A. Softa, Dept. of MSE, University of Pittsburgh, Pittsburgh, PA; Velimir Radmilovic, Department of Physical Metallurgy, University of Belgrade, Belgrade, SERBIA

Manganese-aluminum alloys in the vicinity of the equiaxial composition exhibit an attractive combination of magnetic properties for specific applications in devices involving magnetic fields. The magnetic properties derive from the formation of a metastable Li1.2 intermetallic phase (Li1.2MnAl) characterized by a high uniaxial magnetocrystalline anisotropy with an easy c-axis. Carbon is generally added to stabilize the tetragonal projection on the phase with respect to the formation of the stable phases in the system. The magnetic hysteresis behavior of these permanent magnet alloys is extremely sensitive to the microstructure and defect structure produced during the formation of the Li1.2 phase (Li1.2MnAl) within the parent high-temperature epilayer phase (hep). In this study modern metallographic techniques including high-resolution electron microscopy (HREM) have been applied to elucidate the nature of the phase transformation and evolution of the unique microstructure and defect structure governing the resultant structure-property relationships of these materials. The atomic processes active at the migrating interphase interfaces during transformation are shown to play a critical role in the generation of the so-called twinned microstructures and the profusion of planar defects characteristic of the MnAl1.2-based ferromagnets.

**Y8.4 INFLUENCE OF DISLOCATIONS ON DEUTERIDE FORMATION IN SINGLE CRYSTAL PALLADIUM**

W.C. Chen and Brent J. Heuser, University of Chicago, Dept. of Nuclear, Plasma, and Radiological Engineering, Urbana, IL

The effect of dislocations on deuteride formation in the Pd-D system has been investigated using small-angle neutron scattering (SANS) and in situ transmission electron microscopy (TEM). SANS is extremely sensitive to bulk deuteride formation because deuterium results in greater foreground and lower background signals in metal, capable of providing particle shape, size and orientation information. Deuteride precipitation morphology in well-annealed single crystal Pd and deformed single crystal Pd have been measured with SANS. Dislocations were introduced into the deformed sample by cycling across the hydrostatic miscibility gap. The characteristic response from small, 20-30 Angstrom thick, plate-like Pd has been observed in the SANS measurement of both sample types. We believe these small plates are coherent with the host Pd lattice and not as precursors to the formation of much larger, ten-of-micron thick coherent plate-like crystals. These much larger deuteride plates have a preferred habit plane that depends on sample type, 100 for the well-annealed matrix and 110 for the deformed matrix. The former habit plane is consistent with the maximum strain energy along the elastic-axis of [100] direction. We believe the [110] habit plane is the result of the dislocation substructure influencing the precipitation process. This model is supported by TEM analysis, which indicates a more heterogeneous precipitation process in the deformed sample type. Discussion of our work will focus 1) on the influence of dislocations on bulk deuteride particle morphology and 2) on direct observation of deuteride formation in the presence of dislocations with TEM.

**Y8.5 DISLOCATIONS IN THE FILLED SKUTTERUDITE STRUCTURE**

Jennifer S. Harper and Ronald Gronsky, University of California Berkeley, Dept. of Materials Science and Mineral Engineering, Berkeley, CA

The partially filled skutterudite structure is a candidate thermoelectric material with the capacity for phonon scattering by the decoupled rattling of filling ions. In this transmission electron microscopy investigation of a 1.0% Ce, 1.0% H, 4.9% Ge, 22.8% Co, and 63.1%Sb alloy, both isolated dislocations and arrays of dislocation dipoles are observed. Mechanisms for reducing the strain energy of the expected large Burgers vectors, approximately 8.4, are analyzed, including the possibility of segregation of alloying elements along the dislocation cores.

**Y8.6 DISLOCATION DIPOLE CONFIGURATION IN Gd0.6Ga0.4Nb**

Heterostructures, Y.Q. Wang and Z.H. Wang, School of MSE, Georgia Institute of Technology, Atlanta, GA; T. Brown, A. Brown and G. Muy, Department of Electrical Engineering, Georgia Institute of Technology, Atlanta, GA

Misfit dislocation dipoles, in which two parallel dislocations are separated by about 3.5 nm, have been observed in the solid source MBE Gd0.6Pb0.4Ga0.4 Nb heterostructures (mismatch strain: 0.005%). The dislocations are not exactly located at the interface. They are actually distributed in a zone of 3-5 nm wide in the Ga0.6Pb0.4Ga0.4 Nb epilayer. Furthermore, the distribution of the dislocations along the interface is not uniform. Lengths of up to several tens nm are often dislocation free. Geometrically, the dislocation dipoles are classified into null, extrinsic and intrinsic three types. The dislocations in the dipole are mostly of 60° type. As compared with the theoretical predictions, the two dipole dislocations occupy non-equilibrium stable sites which may result from their interaction with the local strain field. The formation of this special misfit dislocation configuration is believed to be related with the lateral composition modulation in the Ga0.6Pb0.4Ga0.4 Nb epilayer.

**Y8.7 INFLUENCE OF ANTIMONY DOPING ON NANOSCALE ARSENIC CLUSTERS AND DISLOCATION LOOPS**

Low-temperature growth of Gallium Arsenide films, V. V. Chalykh, N.A. Bert, A.E. Romanov, A.A. Surovov, Ioffe Institute, St. Petersburg, Russia; A.L. Kolesnikov, Institute for Problems of Mechanical Engineering, St. Petersburg, Russia; V.V. Peshchanski, M.A. Putyato, B.R. Shemagin, Institute of Semiconductor Physics, Novosibirsk, Russia; P. Werner, Max-Planck Institut für Mikrostrukturphysik, Halle/Saale, Germany

Gallium arsenide grown by molecular-beam epitaxy (MBE) at low temperature (LT) has attracted much attention due to ultrashort carrier lifetime and excellent electrical insulation properties. This material contains a very high arsenic excess which precipitates upon post-growth anneals, so that a large number of arsenic clusters appears in the crystalline GaAs matrix. The As clusters induce rather low strains in the surrounding matrix. On one hand, this enables to easily produce different cluster-containing structures without extended defects such as dislocations, since the self-organized weak deformation fields limit interaction and self-ordering processes in the cluster system. In this paper we show that the strains induced by As clusters can be strongly enhanced when the LT MBE GaAs films are doped with antimony. Arsenic clusters in the Sb doped LT GaAs were found to be surrounded by strong local strains revealed by transmission electron microscopy. The strains originated from Sb incorporation into the clusters and increased with growing cluster size. For critical cluster diameter of 8 nm the yield strength was reduced and dislocation loops were formed at such clusters. The loops were of interstitial type with 1/2 [101] Burgers vector. In the delta-doped samples the clusters were accumulated at Sb delta-layers and the loops lied in [101] planes. The system of a nanoscale cluster with anastropic distortion and attached dislocation loop was considered theoretically taking into account experimentally determined orientation relationships between the cluster and loop in the GaAs matrix, directions of the distortion axes and Burgers vector of the dislocation loop. The theoretically determined dependence of the loop size on the cluster diameter was found to be in a reasonable agreement with that revealed experimentally.

**Y8.8 A NOVEL APPROACH FOR THE COMPLETE REMOVAL OF THREADING DISLOCATIONS FROM Mismatched, HETEROEPITAXIAL LAYERS**

X.G. Zhang, A. Rodriguez, X. Wang, P. Li, F.C. Jain and J.E. Ayers, Electrical and Computer Engineering Department, University of Connecticut, Storrs, CT

Here we demonstrate a novel approach to the complete removal of
threading dislocations from ZnSe on GaAs [101]. This approach, which we call patterned heteroeptaxial processing (PHP), involves post-growth annealing and thermal etching. Post-growth annealing of the substrate pattern has been shown to increase the critical layer thickness for dislocation introduction, the PHP approach allows the complete removal of existing threading dislocations. Epitaxial layers of ZnSe on GaAs grown by MOVPE at $2000-6000 \text{ \degree C}$ were grown, with a microphotoluminescence at $200 \text{ \degree C}$ of $10^2 \text{ cm}^2$-2 threading dislocations. The complete removal of threading dislocations was accomplished by patterning to 70 $\mu\text{m}$ by 70 $\mu\text{m}$ square regions followed by thermal annealing for 30 minutes at temperatures greater than 500$\text{\degree C}$. Neither post-growth annealing nor thermal etching alone had a significant effect, and the effectiveness of this approach diminishes significantly below 500$\text{\degree C}$ so that annealing at 400$\text{\degree C}$ produces no measurable effect. Partial removal of dislocations was observed at temperatures between 400$\text{\degree C}$ and 500$\text{\degree C}$ and the approximate activation energy is consistent with a glide process. We propose that the underlying mechanism for dislocation removal is thermally activated glide of dislocations to the sidewalls of patterned regions, as promoted by sidewall image forces.

**Y8.10 DISLOCATION DENSITY REDUCTION VIA LATERAL EPITAXIAL OVERGROWTH IN GaSb GROWN ON PATTERNED GaAs SUBSTRATES.** Yi, D.M., Hahn, T.F., Kuech, T.F., Dept. of Chemical Engineering, Univ. of Wisconsin, Madison, WI; Inoki, C.K., Harris, D.L., Harris, T.S., Duke, Dept. of Physics, Univ. at Albany, State Univ. of New York, Albany, NY.

Lateral epitaxial overgrowth (LEO) refers to spatially-controlled growth of an amorphous material in which an epilayer is seeded through openings in a mask and grows laterally over the mask from these openings. Recent success in the use of LEO has led to the development of the longest-grown GaN-based lasers. GaSb-based compound semiconductors are of great interest for infrared optoelectronic devices and high-speed electronic devices. Since semi-insulating GaSb substrates are not available, GaSb substrates are normally used in many electronic applications. A principal concern in the growth of GaSb on GaAs substrates is the large, 8% lattice mismatch which leads to a high threading dislocation density on the order of $10^{10}$ cm$^{-2}$. The LEO of GaSb on GaAs substrates is of particular interest because the laterally grown GaSb material could exhibit a reduced threading dislocation density. We present the successful results of LEO of GaSb on patterned GaAs substrates by metallocrystallization chemical vapor deposition. Transmission electron microscopy measurements show that the density of dislocations in the GaSb layer grown on a patterned GaAs substrate with sub-μm openings is less than $10^7$ cm$^{-2}$. Local stress simulation indicates that the local stress is the primary contributor to the dislocation density. Further analysis shows that the GaSb layer becomes more perfect as the opening size decreases, resulting in significant dislocation density reduction.

**Y8.11 MODELING OF PHASE TRANSFORMATION DURING HOMOGENIZATION OF TERNARY ALUMINUM ALLOYS.** Th. Hoferstorfer, K. Greven, A. Ludwig, P.R. Saks, R.W. Achen, Forschungs Institut, Aachen, Germany.

The microstructure determines the most part mechanical properties of complete this is the case especially with age-hardening aluminum alloys. To predict the phase transformation in cast parts and after solidification a sophisticated approach to coupled modeling of various simulation phenomena is presented. This approach couples a diffusion equation solver which considers the online estimation of thermodynamic equilibrium with a macroscopic model for temperature calculation. The macroscopic calculations were performed by means of the in-house 3D-FEM program CASTS. It enables the simulation of the temperature distribution in castings taking into account various initial and boundary conditions. The coupled micro-model predicts the dendrite solidification of ternary alloys. It characterizes important microstructural features like dendrite arm spacing and the amount of fraction eutectic. Effects like solid state lock dislocation, dendrite arm coarsening and tip undercooling are considered. Phase diagram information for a multi-component system is provided on-line by the commercial program ChemApp. To simulate the phase transformation in temperature zones below solidification a homogenization model is used. This model respects the lower diffusion coefficient and shorter diffusion range in solid phases. In order to reduce the calculation time different methods for binary and ternary area are applied. Permanent mould casting and thermal treatment experiments with ternary aluminum alloys are used to validate these models.

**Y8.12 SEGREGATION AT INTERFACES IN AN EVOLVING MICROSTRUCTURE.** Ouf C. Helman and David N. Seidman, Dept. of MSE, Northwestern University, Evanston, IL.

We have shown in previous work that the magnitude of segregation at a grain boundary is influenced by the local stress at the boundary, which can differ for each particular geometric orientation of the boundary. We extend this work to show how these differences are influenced by temperature and chemical potentials of the species involved. In an evolving microstructure, grain boundaries provide lower energy sites for substitutional impurities. As the absolute amount of grain boundary area changes in an evolving microstructure, the chemical potential of these impurities will change depending on their excess concentration at the boundaries. Through Monte Carlo simulations, we explore the structure and the thermodynamics of segregation at grain boundaries. The local stress effect on the equilibrium concentration of the different boundary geometries is found to change as a function of the chemical potential, and segregation is shown to influence the evolution of grain structure by influencing the energy of different boundary types. This research is supported by the National Science Foundation, Division of Materials Research, Grant DMR-972896, Bruce McDonald, Grant Officer.

**Y8.13 THE EFFECTS OF A NEW GRAIN BOUNDARY PHASE IN Ni-Al ALLOY.** Y.L. Chin, A.H. W. Ng, Dept. of Mechanical Engineering, The Univ. of Hong Kong, Hong Kong SAR, PR China.

In a boron-doped nickel-aluminum alloy, which shows higher ductility and toughness than the boron-free one, a new phase has been identified along grain boundaries with conventional transmission electron microscopy (TEM). This phase is identified to be of Cu$_3$Ga$_2$Sb$_5$ type structure with unit lattice parameter of $10.48 \text{ \AA}$, which is approximately three times that of NiAl or nickel. This grain boundary precipitate is found to be coherent with one grain. The chemical composition of this grain boundary precipitate is determined by energy dispersive x-ray spectroscopy (EDX) and parallel electron energy loss spectroscopy (PEELS) respectively. The deformation mechanism of this grain boundary precipitate is investigated on yttrium-strengthened specimen. The deformation mechanism of this grain boundary precipitate is investigated on yttrium-strengthened specimen. The deformation mechanism of this grain boundary precipitate is investigated on yttrium-strengthened specimen. The deformation mechanism of this grain boundary precipitate is investigated on yttrium-strengthened specimen. The deformation mechanism of this grain boundary precipitate is investigated on yttrium-strengthened specimen.

**Y8.14 INTERFACE STRUCTURE IN FERRITIC/AUSTENITIC STAINLESS STEEL BICRYSTALS.** A. Taisse, B. Dévamps, Laboratoire de Chimie Métallurgique des Terres Rares, UPR 208 du
INTERACTIONS BETWEEN PARTICLES AND INTERFACES: AN IMPORTANT ROLE IN THE PHASE TRANSITIONS IN MATERIALS

INTRODUCTION

Interfaces are important in many physical processes, such as phase transitions, transport phenomena, and the mechanical properties of materials. The interaction between particles and interfaces is crucial in determining the behavior of materials under various conditions.

RESULTS

1. Interactions between particles and interfaces play a significant role in the phase transitions in materials. These interactions can affect the stability, dynamics, and energy of the system.

2. The mechanical properties of materials are strongly influenced by the presence of interfaces. The strength and stiffness of composite materials, for example, are determined by the interface properties.

3. The transport phenomena in materials, such as electrical conductivity and thermal conductivity, are also affected by the interactions between particles and interfaces.

4. The phase transitions in materials are governed by the interplay between the particles and the interfaces. The energy landscape is modified by the presence of interfaces, leading to different phase transitions.

CONCLUSIONS

1. The interactions between particles and interfaces are important in determining the behavior of materials.

2. The mechanical, transport, and phase transition properties of materials are strongly influenced by the interface properties.

3. Understanding the interactions between particles and interfaces is essential for the development of new materials with desired properties.

REFERENCES


Y8.22 COAGULATING KINETICS OF COHESIVE PRECIPITATES
DEPENDENCE ON VOLUME FRACTION. Ven Kothiyavani,
L.Q. Chen, Department of MSE, Pennsylvania State University,
University Park, PA.

Rate of coagulating precipitates have been shown to depend on
volume fraction for many alloy systems. The coagulation rate
dependence on volume fraction for ordered \( \gamma' \) precipitates in Ni-Al
alloys, with significant lattice misfit, is not very clear. Experimental
results on Ni-44\%Al. We try to extract the coagulating kinetics dependence on volume fraction of \( \gamma' \) precipitates
in Ni-Al binary alloy, using continuum phase-field model in two-dimension(2D). The results of our simulation are presented here.

Y8.23 INTERACTION OF SLIP BANDS WITH GRAIN BOUNDARY - IN
SITU TEM OBSERVATION. J. Gempeler1, A. Jacquès1, M
Jureček2, T. Vysoký2, A. Gemberle1, Z. Zábořil4.1 Institute of
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Mathematics and Physics, Charles University, Prague 2. 2Laboratoire de
Physique des Matériaux, Ecole des Mines, Cedex, FRANCE.

Previous studies of dislocation interactions with grain boundaries
(GBs) on quasimicroscopic scale by in situ SR X-ray topography on
Fe-4m\%Si symmetric nearly 23 \([110]/[70,5] \) bicrystals have shown that
these GBs form strong barriers for the slip transmission even for the
same slip geometries in both grains. A repetitive image force,
stresses exerted by dislocations accumulated at the heads of individual
slip bands and local structure of GB affect the transmission.

Investigations by in situ TEM tension deformation were performed to
elucidate these observations. Symmetrical bicrystals with near 23 misorientation and the GB plane \((\mathbf{T}_1)/[\mathbf{T}_1]\) had the deviation from the exact coincidence in one-degree range. The specimens had the form of plane 7×5×4 mm and thickness 0.02 mm. The boundary passed through the hole in the centre. The specimen normals were \([\mathbf{B}_1]/[\mathbf{B}_1]\) and \([\mathbf{B}_2]/[\mathbf{B}_2]\) for the tensile axes were chosen to perform slip transmission of dislocations with both primary Burgers vectors \((\mathbf{B}_1) / [\mathbf{B}_1] \) and slip planes parallel in the
two grains. The specimens were observed during straining under
bright field diffraction conditions using different deflecting vectors in
each grain. The observations were registered on videotape. After the
experiment detailed examinations of samples post mortem were
performed using two-beam bright and dark field imaging in various
reflections.

In no case the propagation of slip caused by primary slip dislocations
was observed. When tensile axis is lying in the GB plane the slip
dislocations of tertiary slip system enter the GB, interact with GB
dislocations and dislocations of secondary slip system are generated in
the second grain. When the angle between the slip plane and GB is
about 25° the primary slip dislocations, whose Burgers vector belongs
to the GB plane, cross slip and follow the GB plane. Primary slip
dislocations are formed in one grain and a new subgrain boundary is
formed in the other grain when the angle between the slip plane and GB is
say 40° the dense set of GB dislocations, which crosses slip
dislocations, prevents the transmission of slip dislocations across the
GB. The angle between the slip plane and GB plane plays an
important role in slip propagation across the GB. The larger is the
angle, the easier is the slip propagation. An unusual deformation mode
has been observed for one orientation of the tensile axis and the
GB. The financial support of GA of CR (the grant contract
202/98/1381) and of FFC (No. 477) is acknowledged.

Y8.24 GRAIN GROWTH IN ANISOTROPIC SYSTEMS WITH LARGE
GRAIN BOUNDARY MISORIENTATIONS AND EFFECT OF
PORE DRAG ON GRAIN BOUNDARY MOBILITY. A. Kuehni,
Y. Wang and Bruce R. Patton, Ohio State University, Columbus, OH.

Domain dynamics and morphology of a polycrystalline system with
anisotropic grain boundary energy and mobility is investigated using the
Phase Field Model. In contrast to previous simulations where the
small misorientation limit was investigated, we discuss in this work
the case of large misorientations and the influence of special
boundaries. Energy and mobility data obtained from MD simulations
are used as the input parameters. Kinetics of grain growth as well as a
variety of topological and morphological features are analyzed and
compared to the small misorientation case.

Y8.25 EFFECT OF PORE DRAG ON GRAIN BOUNDARY MOBILITY.
Ning Ma, Shen Chen and Yunzhi Wang, The Ohio State University,
Department of MSE, Columbus, OH.

The effect of pore drag on grain boundary mobility is investigated
using a diffusion interface phase field model. The model takes into
account various diffusion mechanisms without imposing any priori
constraint on the geometry of the interacting pores and grain
boundaries. The grain boundary mobility has been characterized as a
function of the driving force for the boundary motion, the ratio of
surface vs. grain boundary diffusion, and the pore size and inter-pore
spacings. Computer simulations results illustrating the effect of these
parameters on grain boundary mobility as well as on the
morphology of the interacting grain boundary and pores will be
discussed.

Y8.26 NUCLEATION OF PORTEVIN-LE CHÂTELIER BANDS IN
PLASTICALLY DEFORMING ALLOYS. P. Sipilišnìk, Lab of
Mechanics & Metals, Aristotle University of Thessaloniki, Thessaloniki,
Greece; M. Zaiser, Max-Planck Inst fur Metallforschung, Inst fur
Physik, Stuttgart, Germany; P. Hakner, TU Braunschweig, Inst fur
Metallphysik & Nukleare Festkörperphysik, Braunschweig,
Germany; E.C. Affinita, Lab of Mechanics & Metals, Aristotle University
of Thessaloniki, Thessaloniki, Greece.

The Portevin-Le Chatelier (PLC) effect observed in plastically
deforming alloys is associated with the repeated unpinning of
dislocations from, and the recapture by, solute atoms. This process
is known as dynamic strain aging (DSA). Using a recent model of the
coupled dynamics of DSA and strain hardening as proposed in [1], the
influence of intrinsic fluctuations of the dislocation velocities on the
nucleation of PLC bands is investigated. It is demonstrated that
fluctuations in the solute pinning strength (which in previous theories
of the PLC effect [2] was considered to be a 'fixed' variable) may
trigger the nucleation of localized deformation bands. The rate of
nucleation is derived as a function of stress, strain and materials
parameters. Implications for the shape of stress-strain curves and
analogies with other strain-rate softening phenomena are discussed.

Y8.27 ATOMIC-SCALE MODELLING OF DISLOCATIONS MOVEMENT
IN 2D SYSTEMS: BRITTLE AND DUCTILE REGIMES.
M. Roberts, K. Kaski and V. Mustonen, Helsinki University of Technology,
Laboratory of Computational Engineering, Espoo, Finland.

In this study strained 2D systems have been modelled at the atomic
scale to investigate the role of dislocations in brittle-ductile transition.
The modelling is done interactively using Molecular Dynamics method
and a graphical user interface which allow us to visualize the
dynamical evolution of the system, and track automatically the
nucleation and movement of all the dislocations in the system. In the
model the interaction potential is a hybrid of Lennard-Jones (LJ)
potential and Embedded Atom Model (EAM) potential. These
potentials are coupled with a weight parameter that allows us to change
the character of the system to resemble that of a brittle material
(pure LJ system) or to resemble that of a ductile material
(pure EAM system). The dynamics of a single dislocation under strain
is studied as a function of the coupling parameter to yield insight to the
dislocation movement when brittle-ductile transition takes place. In
addition we have examined the evolution of a cross slip loop,
giving special attention to the movement of the dislocation nucleated at the
tip.

SESSION Y9: INTERFACE ANISOTROPY II
Chairs: Michael W. Finnis and Douglas L. Medlin
Thursday Morning, November 30, 2000
Independence E (Sheraton)

8:30 AM *Y9.1 A PHASE FIELD MODEL FOR SYSTEMS WITH HIGHLY
ANISOTROPIC SURFACE ENERGY. J.J. Eglington, P.W. Voorhees,
Dept of MSE, Northwestern Univ, Evanston, IL

Interfacial energies in many materials are strongly anisotropic. In such
cases the Wulff shape changes possess missing orientations, or corners
and edges. Semiconductor quantum dots is one example of a system
in which growing phases possess strongly anisotropic surface energies.
The challenge in computing the evolution of such surfaces is that the
equations defining the evolution of the surface can become ill posed.
The solutions of the equations can, thus, be a function of the solution
technique itself. To avoid these problems in the context of a sharp
interface description, it is necessary to track explicitly the location of
the corners and edges. A computationally efficient method to circumvent
these problems we have developed a phase field method for computing
the evolution of surfaces with missing orientations. The method has the
advantages that it is stable and does not require that the
location of corners be known. Examples will be given of the
evolution of surfaces with initial shapes that include missing
orientations, the evolution of lattice mismatched thin films, and
quantum dot formation during heteroepitaxy on planar and patterned
substrates.
9:00 AM  #Y0.2
THE ROLE OF EDGES AND LEDGES IN THE EQUILIBRIUM SHAPE OF SOLID AND LIQUID PRECIPITATES
Ulrich Dahmen, Heike Gabrisch, National Center for Electron Microscopy, LBNL, UC Berkeley, CA; Erik Johnson, Center for Electron Microscopy, Nihon Bohr Institute, University of Copenhagen, DENMARK.

The equilibrium shape of small Pb inclusions in Al has been investigated by high resolution and in situ electron microscopy. Solid inclusions exhibit equilibrium shapes that are fully faceted, follow a sequence of magic sizes, and whose misorientation depends on size. This behavior can be understood as a result of their oscillatory residual strain energy, an energy term that is found to be only elastic in nature. Liquid inclusions display shapes that are partially faceted, and whose facet size and aspect ratio depend on size, temperature and thermal history. Shape equilibration is shown to be kinetically limited by the need to nucleate edges in order to reach the true equilibrium shape. Analysis of the size dependent shape evolution indicates a roughening transition at about 550°C. The observations described in this work give direct evidence of the overriding effect of edges and edges in the equilibrium shape and the approach to equilibrium when the inclusion size is in the range of a few nanometers. This work is supported by the Director, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

10:30 AM  #Y0.3
PHASE DIAGRAM, INTERFACIAL FREE ENERGIES, AND TEMPERATURE DEPENDENCE OF COHERENT MICROSTRUCTURE IN Al-Sc ALLOYS. Viivi M. Rantala, Dept. of Thin Film and Interface Science, Sodin National Laboratories, Livermore, CA; Mark Astra, Dept. of MSE, Northern Univ., Evanston, IL.

Thermodynamic properties of anisotropic microstructures in Al-Sc alloys are studied using first-principles local-density-functional calculations. We find that vibrational entropy plays a very important role in this system, increasing the solubility of Sc in FCC Al matrix by a factor of thirty. Using atomic Monte Carlo simulations we study shapes of coherent precipitates of the intermetallic (L1_2) AlSc phase in Al matrix as functions of precipitate size and temperature. We find a strong preference for forming cubic Al12Sc precipitates, which remain faceted up to the melting point. Effect of vibrational entropy on interfacial free energies and precipitate shapes is discussed.

SESSION Y10: INTERFACIAL CHEMISTRY
Chair: Michael W. Finnis and Douglas L. Medlin
Thursday Morning, November 30, 2000
Independence E (Sheraton)

10:15 AM  #Y10.1
STOICHIOMETRY AT THE OXIDE-METAL INTERFACE.
Michael W. Finnis, Ali Alwi, Iskander G. Baigunm, Queen’s University of Belfast, Atomic Simulation Group, Belfast, UNITED KINGDOM

The growth of oxide precipitates in metals, or of oxide scales on metals, depends on the detailed structure and stoichiometry at the interface. The determination of the stoichiometry can be viewed as a problem of whether or not oxygen would segregate to or desegregate from a reference interface. The segregation of other elements may be important too, such as sulfur in the growth and adhesion of oxide scales. An equivalent formulation of the problem is to ask whether the carbon free energy as a function of stoichiometry. We outline a method for doing such calculations at the atom scale, illustrating it by discussing the relative free energies of variously terminated Si(001)-aluminum (0001) interfaces which were obtained from first-principles, plane-wave pseudopotential calculations[1]/[2]/[3] I G. Baigunm, A Alwi and M.W. Finnis, Phys. Rev. B, 61, to appear (tentatively in August), (2000).

10:45 AM  #Y10.2
NANOSCALE STRUCTURE AND CHEMISTRY OF α-IRON / MOLYBDENUM NITRIDE HETEROEPHASE INTERFACES.
Dexter Johnson and David N. Seidman, Northwestern University, Department of MSE, Evanston, IL.

We are studying heterophase interfaces between molybdenum nitride precipitates and an α-iron matrix in nanoscale by electron and atom-probe field ion microscopies. Internal nitridation is achieved by annealing specimen of Fe +.3%Mo +.4at%Cr +.7at% in an NH3/H2 atmosphere. Nitridation at temperatures between 550 and 650°C creates molybdenum nitride precipitates with a variety of morphologies and therefore a variety of heterogeneous interfaces. At lower temperatures, thin platelet-shaped precipitates a few atomic layers thick form, while nitridation at higher temperatures results preferentially in a corner microstructure containing thin platelets and spherical-shaped precipitates. A higher level of Sb segregation is observed at the heterogeneous interfaces of the larger and thicker precipitates. The loss of coherence that is the generation of misfit dislocations, is significant for the formation of these more massive precipitates. The relation between misfit dislocations at these heterogeneous interfaces and Sb segregation is discussed.

Research supported by the National Science Foundation (Division of Materials Research), the Deutsche Forschungsgemeinschaft, and the Alexander von Humboldt Stiftung through the Max-Planck-Research Prize of D.N.S.

11:00 AM  #Y10.3
COMPARISON OF THE 25 [310]/[0001] SYMMETRIC TILT GRAIN BOUNDARY IN COPPER, DOPED COPPER, AND DOPED COPPER. Jürgen M. Plata, Geoffrey H. Campbell, Wayne E. King, Chemistry and Materials Science Directorate, University of California, Lawrence Livermore National Laboratory, Livermore, CA; Stephen M. Foiles, Computational Materials Science Department, Sandia National Laboratories, Livermore, CA.

We have chosen a model grain boundary to investigate the size effect on segregation of an impurity to distinct sites in the boundary. Specifically, we used copper segregation in an aluminum and silver (85.75/14.25 composition) in a copper [310]/[0001] symmetric tilt grain boundary (STGB) in combination with image simulation. We also used local-site segregation to validate the predictions of the EAM model. Focal-series reconstruction can provide not only detailed information on the atomic structure, but it can also provide chemical information related to the projected potential (atomic number) of the elements under investigation. This makes it possible to compare reconstructed images to images obtained with Z-contrast investigations. Using analytical electron microscopy the amount of copper (and likewise silver) was measured, and the electronic structure of the Cu atoms in and at the boundary were investigated by means of ELNES of the Cu-L2,3 edge. We will present and compare our results for the different metals with the modeled systems, and we will discuss our observations with respect to earlier results. This work was performed under the auspices of the U.S. Department of Energy Office of Basic Energy Sciences by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

11:15 AM  #Y10.4
CHARACTERIZATION OF LAMELLAR INTERFACES FOR A PST-TAI1 ALLOY BY AN ANALYTICAL SCANNING TRANS- MISSION ELECTRON MICROSCOPE. Wei Zhang and David E. Luzni, University of Pennsylvania, Department of MSE, Philadelphia, PA.

Poly-synthetically-twinned (PST) TAI1 with a gamma-alf2 lamellar structure has the potential for application in the aircraft and automotive industries due to its high specific strength, and a high oxidation and creep resistance at elevated temperatures. Additions of certain ternary elements to the binary TAI1 system appear to improve the ductility of the material from room to high-temperatures, which will facilitate its scale-up for applications. In this article, the microstructural features of lamellar interfaces and the interface behavior are investigated using electron microscopy. A binary TAI1 (Al-19.3% at.%) and relaxed ternary TAI1 X 0.6% at. [X = Ni, Cu, Mn, W, and Ta] alloys are characterized by high-resolution (JEOL 4000F) and field emission analytical transmission electron microscopy (JEOL 4000F), coupled with energy dispersive X-ray spectroscopy, elemental mapping and line-scan techniques. TEM samples are prepared from the TAI1 single crystal with a 6° tilt, followed by a flattening-zone directional solidification technique. Swings, stacking faults, and defects at interfaces, as well as the segregation of ternary elements to the lamellar boundaries, are characterized.

11:30 AM  #Y10.5
ATOMIC AND ELECTRONIC STRUCTURE OF HIGH PURITY Si CRYSTAL BOUNDARY. David N. Seidman, Dexter Johnson, The Univ of Tokyo, Dept of Material Engineering, Tokyo, JAPAN.
Grain boundary atomic structure of a high purity silicon carbide (mainly 6H-SiC) was determined by an atom-resolution high voltage transmission electron microscopy (HREM) at the Scherrer defocus condition. We can now distinguish atomic sites of Si and C in the grain boundary from the image contrast; Si atomic columns appear in a darker spot and C atomic columns appear in a thinner spot. Mainly observed boundary was parallel to [0001] plane of one crystal and to [11-20] plane of the other, rotated by 70.5 degrees around [11-20] axis. A structural unit of this boundary consisted of 5.6-6.5-membered rings. In the 5-membered rings, Si faced to each other (Si to C). Only the atomic pairs between the 5-membered ring and the 2-membered ring was Si-Si. Measured Si-Si distance corresponded to nearly 120% of nearest neighbor distance of SiC crystal. Since the Si-Si distance in the Si crystal is 122% of Si-C distance, it can be said that the measured value is very close to that of Si crystal even in the SiC boundary. Each structural unit had two three-coordinated atoms. The one located in the 2-membered ring and the other was in the 5-membered ring. The atomic species of the three-coordinated atoms were definitely determined to be carbon from the image contrast. Electronic structure of the boundary was investigated by both first-principles density functional theory (DFT) and the first-principles molecular dynamics method.

SESSION XI: INTERFACE AND DISLOCATION INTERACTION

Chairs: Mark Aindow and Douglas L. Medlin

Thursday Afternoon, November 30, 2000

Independence E (Sheraton)

1:30 P M  *XI1.1

INTERFACE-LINE-DEFECT MECHANISMS IN SHAPE-MEMORY ALLOYS: A CASE STUDY

M.C. Lees, M.E. Paasch, M.B. Cottrell, and P. Fox, Department of Engineering, University of Liverpool, Brownlow Hill, Liverpool, UNITED KINGDOM.

Alloys which exhibit shape-memory (SM) and super-elastic (SE) behaviour are extensively used in a wide range of applications. The thermomechanical properties of these materials rely on easy motion of martensitic and twin interfaces. This motion is accompanied by shear-dominated and planar dislocation deformation in the two types of interfaces respectively, and is diffusionless in both cases. Moreover, there is considerable experimental evidence that the passage of interfacial dislocations along these interfaces is the mechanism by which the interfacial-dislocation and interface migration are coupled together. The object of the present paper is to review our theoretical understanding of interfacial defects in the context of SM and SE materials and compare this with experimental observations. In particular, it will be shown that defect mechanisms which couple deformation with interface migration and which are also diffusionless can only arise in special crystallographic circumstances. This appreciation offers mechanistic insight into the modelling of martensitic transformations, which has been developed phenomenologically in earlier treatments. An important aspect of modelling in terms of defects is to consider the interaction of lattice-invariant deformation in a martensite phase with interfacial transformations, which we propose to demonstrate. In such interactions require zero diffusional flux of material. In addition, the physical attributes of transformation and twinning dislocations which endow high mobility will be discussed, and also the influence of interfacial defect mechanisms on the evolution of microstructure in these materials which arises in response to applied stress and/or changes of temperature will be outlined.

2:00 P M  *XI1.2

HREM STUDY OF INTERFACES IN A DUELPLEX STAINLESS STEEL

Hsinheng Jiao, Malcolm Hall, Univ of Birmingham, School of Metallurgy and Materials, Birmingham, UNITED KINGDOM; Robert Pond, Dept of Metallurgy and Materials, University of Liverpool, UNITED KINGDOM; Mark Aindow, Univ of Connecticut, Dep of Metallurgy and Materials Engineering, Institute of Materials Science, Boston, CT, USA.

We have used Zeron-100, a commercial duplex stainless steel, as a model system to investigate the interfacial structure between FCC and BCC crystal structures. After a series of heat treatments, a Widmanstätten structure with clearly defined interfaces was obtained. Precise determination of the orientation relationship (OR) between gamma (FCC) and alpha (BCC) showed it to be near Kurdjumov-Sachs (K-S) with a misorientation of 1.4 degrees between [011]alpha and [11-20]gamma, and 0.3 degrees between [11-1]alpha and [011]gamma. The details of the interfacial structure and defect content were studied by conventional TEM and HREM techniques. The precipitated gamma particles exhibited well-defined interfacial facets on (111)gamma and (221)gamma. Both of these interfaces were semiconductor with periodic line defects aligned parallel to the growth direction of the particle (about 5 degrees away from (111)alpha). The interfacial line defects were characterized by using circuit mapping procedures to analyze HREM images obtained with an edge-on, and comparing these data with what we would expect on the basis of the topological theory of interfacial defects. In this paper, we will show that by using these results together with a suitable crystal structure, we can account for the misorientation from the K-S or measured experimentally. The role of such interfacial defects in the development of Widmanstätten-type microstructures will be discussed.

2:15 PM  *XI1.3

SLIDING BEHAVIOUR OF SYMMETRIC TILT BOUNDARIES WITH SPECIAL, NEAR-SPECIAL AND NON-SPECIAL MISORIENTATIONS IN ZINC BICRYSTALS. Askar Sheikd-Ali Jerzy Sempier, Dept of Metallurgical Engineering, McGill University, Montreal, QC, CANADA.

Observations of grain boundary sliding along symmetric tilt coincidence S1=9112 and three boundaries deviated at different angles from coincidence misorientation have been made in zinc bicrystals. The coincidence boundary and boundaries whose rotation does not exceed approximately degrees slide and migrate in a coupled manner predicted by the DSC dislocation model. The boundary whose deviation exceeded approx 5 degrees slides without migration and with a significantly lower rate in contrast to the previous boundaries except the coincidence one. The sliding along the coincidence boundary is activated at higher stresses only in the presence of intragranular slip. These results enable to distinguish special, near-special and general boundaries. It is emphasized that the ability of the boundary to slide and migrate in a fixed ratio is an important criterion for its specialness.

2:30 PM  *XI1.4

THE EFFECT OF EXTENDED SUPERDISLOCATION / DOMAIN BOUNDARY INTERACTIONS IN ORDERED INTERMETALLIC COMPOUNDS. T.S. Rong, J. P. Jones, School of Metallurgy and Materials, Univ of Birmingham, Birmingham, UNITED KINGDOM; M. Aindow, Dept of Metallurgy and Materials Engineering, Univ of Connecticut, Storrs, CT.

It has been known for many years that the presence of a distribution of domain boundaries in crystals with ordered superlattice structures can affect both the separation of glissile superpartial dislocations and the yield stress [1-5]. In our work we have developed a new model for these effects based on the details of the interactions between the domain boundaries and glissile extended superdislocations. In this model, we incorporate the effects of the thin band of perfect crystal that arises when coupled superpartial dislocations straddle a domain boundary, and the additional domain boundary we created once the whole superdislocation has passed through. In this paper we will present an overview of this model. It will be shown that these effects are included then, in an ordered phase containing many domains, we would expect the equilibrium separation of the coupled superpartial dislocations to vary significantly with domain size. In addition, the fact that one would expect gives a better match to published experimental data than is predicted by previous models. It will be also shown that these effects can change the way in which yield stress varies with domain size and that the variation that one would expect gives a much better match to published experimental data than is predicted by previous models.

3:00 PM  *XI1.5

"DISLOCATION-GRANULAR INTERACTION" IN NICKEL BICRYSTALS AND EVOLUTION OF THE RESULTING DEFECTS UNDER THERMAL TREATMENT. Lucie Boisseau, Sophie Pauzi, Université Paris XI, LEMHT, Orsay, FRANCE; Brigitte Décraps, CNRS, LCMFR, Thiais, FRANCE; Jany Blanquet, CE/A, DRFMC, Grenoble, FRANCE.

The interactions between lattice dislocations and grain boundaries (GBs) have been studied in nickel bicrystals grown by solidification along the <111> axis. Three types of GBs, according to their energy, have been investigated: singular (111), near (311) and general near (311) GBs. The experiments were performed by Transmission Electron Microscopy (TEM) using a set of techniques: conventional bright and dark field, weak beam, in situ and high resolution microscopy.

Dislocation transmission from one crystal to the other has been only observed for GB (111) GB. It consists in a disconnection within the GB of the trapped lattice dislocation followed by the emission of one partials at the nearest neighbour crystal. But, most often, the absorbed lattice dislocations or extrinsic grain boundary dislocations (EBDs) relax with the intrinsic dislocation network giving rise to complex
configurations. The evolutions with time and upon thermal treatment of these configurations have been followed by in situ TEM. The results show that the processes and the kinetics differ with the type of GBs. They have been analyzed by comparison with the existing theoretical models for EGBD accommodation. Their interpretation rests on the knowledge of the processes at the atomic GB structure level and thus requires complementary HRTEM investigations.

4:00 P.M. Y11.6

DELOCALIZATION DYNAMICS IN INTERMETALLIC, OXIDE DISPERSION STRENGTHENED (ODS) AND QUASICRYSTALLINE ALLOYS. Ulrich Messerschmidt, Martin Bartsch, Max Planck Institute of Microstructure Physics, Halle (Saale), Germany.

In situ straining experiments in a high-voltage electron microscope allow the observation of the dynamic behaviour of individual dislocations. Such experiments have been performed on the intermetallics NiAl, TiAl, and MoSi2, the ODS alloys INCOLOY MA956 and INCONEL MA754, and Al-Pd-Mn quasicrystals up to 1150°C. The behaviour of dislocations under load can be characterized by their geometrical shape and the dynamic behaviour, i.e. the degree of jerking of their motion. Both are specific of the different mechanisms controlling the dislocation mobility. Straight dislocations moving viscoplastically are consistent with lattice friction mechanisms like the Peierls mechanism or the existence of non-planar dislocation cores. Bowed-out dislocation segments and a jerky motion on a mesoscopic scale point to the motion of localized obstacles, where the barreling is frequently controlled by the line tension. There are many similarities in the dynamic behaviour of dislocations in different materials. In intermetallic alloys, a transition occurs between low temperature mechanisms like the pinning by small precipitates or jogs or the Peierls mechanism and a viscous motion in the temperature range of the flow stress anomaly. The viscous motion at high temperatures can be explained by diffusion processes in the dislocation cores, where the diffusion species can be quite different, alloying components or intrinsic point defects like vacancies and interstitial defects existing in the lattice or only in the dislocation cores. It may also be a cooperative climb between partial dislocations separated by a climb dislocation. Viscous motion occurs also in quasicrystals and is controlled by the intrinsic cluster structure of these materials. A case of particular interest is the superposition of a viscous motion and the pinning by localized obstacles as it appears in oxide dispersion strengthened alloys. The relation between the dislocation dynamics and the strain rate sensitivity of the flow stress is discussed for the different materials.

4:30 P.M. Y11.7

STRESS DRIVEN PHASE TRANSFORMATIONS AND RECRYSTALLIZATION PROCESSES IN TWO-PHASE TITANIUM ALUMINIDE ALLOYS. Fritz Appel and Michael Oehring, GKSS Research Centre Geesthacht, Inst for Materials Research, Geesthacht, Germany.

High temperature strength and structural stability are critical issues for engineering applications of gamma-phase titanium aluminides. The mechanisms controlling these properties are not yet fully understood, partly due to the wide variety and complexity of microstructures that can be established in these alloys. This holds particularly for stress induced structural changes due to phase transformations and recrystallization, which might be important for long-term creep at relatively low stresses. The paper presents a high resolution electron microscope study of diffusion assisted creep processes in a lamellar alpha 2(Ti3Al) gamma(TiAl) alloy, which involve phase transformations and recrystallization. The observed mechanisms were found to be closely related to the atomic structure of lamellar interfaces and are probably driven by a non-equilibrium of the phase composition. The processes finally end up in the formation of gamma grains and a complete conversion of the lamellar morphology to a fine spheroidized microstructure.

4:45 P.M. Y11.8

DISSOCIATION OF AND 90° PHASE FORMATION IN A HIGH ANGLE GRAIN BOUNDARY VIA SEPARATION OF INTERFACIAL DISLOCATIONS. Stephen M. Riles, Sandia National Laboratories, Albuquerque, NM; Doug L. Medlin, Sandia National Laboratories, Livermore, CA.

A film grown on a Ge(001) substrate have a [110] texture and develop a domain structure with two crystal orientations related by a 90°-degree rotation. The boundaries between the domains are observed to form 111/121 boundary facets separated by dislocations localized at boundary steps. The facets are observed to have a dissociated structure with a region of 90° phase at the boundary. This is similar to the 90° phase formation observed previously for 221 boundaries. However, in this case the dissociation is observed to occur at a high angle boundary which has approximately a 221 orientation. The structure of this boundary has been computed using atomistic simulations based on the embedded atom method. The simulations confirm the dissociated nature of the boundary and are in good agreement with the experimental observations. The dissociated structure of the boundary will be analyzed in terms of a generalization of a dislocation model proposed earlier to describe the 221 case.