SYMPOSIUM Y

Influences of Interface and Dislocation Behavior on Microstructure Evolution

November 27 – 30, 2000

Chairs

Mark Aindow
Metallurgy & Matls Engr Dept
Univ of Connecticut
97 North Eagleville Rd
Storrs, CT 06269-3136
860-486-2644

Mark Asta
Dept MS&E
Northwestern Univ
Evanston, IL 60208-3108
847-491-5940

Michael V. Glazov
Ctr for Material Mech & Microstructure
Alcoa Technical Center
Bldg C
Alcoa Center, PA 15069-0001
724-337-2847

Douglas Medlin
Thin Film & Interface Science Dept.
Sandia Natl Labs
MS 9161
Livermore, CA 94551
925-294-2825

Anthony D. Rollett
Dept of MS&E
Carnegie Mellon Univ
Wean Hall 4315
Pittsburgh, PA 15213-3890
412-268-3177

Michael Zaiser
Max Planck Inst für Metallforschung
Stuttgart, D-70569 GERMANY
49-711-6891907

Symposium Support

†E.A. Fischione Instruments, Inc.
†FEI Company (Micrion/FE/Philips)
Gatan, Inc.
†JEOL USA, Inc.
†Oxford Instruments America, Inc.
TSL Inc.

†2000 Fall Exhibitor

**Proceedings published as Volume 652
of the Materials Research Society
Symposium Proceedings Series.**

* Invited paper

SESSION Y1: INTERFACE MOTION I – COLLECTIVE GRAIN MOTION
Chairs: Mark D. Asta and Anthony D. Rollett
Monday Morning, November 27, 2000
Independence E (Sheraton)

8:30 AM *Y1.1
INTERFACE DYNAMICS: A NOVEL TOOL FOR MICRO-STRUCTURAL CONTROL. Günter Gottstein, Dmitri A. Molodov, Myrjam Winning, Institut für Metallkunde und Metallphysik, RWTH Aachen, GERMANY; Lasar S. Shvindlerman, Institute of Solid State Physics, Russian Academy of Science, Chernogolovka, RUSSIA.

The microstructural restoration 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 biassed at desire if interface motion can be effectively influenced. We will present evidence that it is possible to affect the motion of grain boundaries by a variety of externally controlled driving forces. Albeit small 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 selection. 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 MIGRATION IN POLYCRYSTALLINE MATERIALS. J.K. Farrer, N. Ravishankar, 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.

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 $CaAl_2Si_2O_8$, 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 MICROLAMINATES. A.C. Lewis, A.B. Mann, D. Van Heerden, T.P. Weihs, Johns Hopkins University, Dept of MS&E, 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 grooving and the pinch-off of individual layers. Such samples, when exposed to high temperatures, develop grooves where grain boundaries meet the interfaces between layers. The depths of the grooves are controlled by the ratios of grain boundary and interfacial free energies, γ_{gb}/γ_{int}. If γ_{gb} is much smaller than γ_{int} then there is little grooving at grain boundary-interface junctions and the layering is stable. If γ_{gb} 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 pinch-off at the grain boundary. This pinch-off destroys the layering and eventually leads to a gross coarsening of the microstructure. When one of the layers in the microlaminate is designed to provide creep resistance or strength, pinch-off of that layer is extremely detrimental to the material's mechanical performance. Because microstructural stability is thus critical to performance, the ability to understand and/or predict the stability of microlaminates is a necessary tool. An existing model of this capillarity driven breakdown requires the interfacial free energies, γ_{gb} and γ_{int} , as input parameters. Both biaxial and uniaxial zero creep tests have been used in conjunction with transmission electron microscopy to measure these interfacial energies in Ag/Ni and Nb/Nb_5Si_3 microlaminates. The measured energies are then used to explain the onset of instabilities and the eventual breakdown of layering in Ag/Ni multilayers on sapphire substrates as well as in free-standing Nb/Nb_5Si_3 microlaminates.

10:00 AM *Y1.4
MODELING THE FORMATION OF GRAIN BOUNDARIES VIA COLLISION AND THEIR SUBSEQUENT EVOLUTION USING A PHASE FIELD METHOD. James A. Warren, Alexander Lobkovsky, National Institute of Standards and Technology, Gaithersburg, MD; Ryo Kobayashi, Hokkaido University, Sapporo, JAPAN; W. Craig Carter, Massachusetts Institute of Technology, Cambridge, MA.

We present a new model of the solidification of arbitrarily 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
MESOSCALE SIMULATION OF GRAIN GROWTH.
David Kinderlehrer, Florin Manolache, Irene Livshits, Shlomo Ta'asan, Department of Mathematical Sciences, Carnegie Mellon University, Pittsburgh, PA.

The simulation of curvature 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 balance equation imposed at triple junctions. We discuss several novel features of our apporach 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 grains (e.g., 70,000) 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 histogram of relative area population as it changes through the simulation. We do not use this data to seek the best distribution, like Hillert, Rayleigh, or lognormal, for a discussion see (*). 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 simulations of large metastable systems. (*)Mullins, W. W. (1998). "Grain growth of uniform boundaries with scaling." Acta materiala 46(17): 6219-6226

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, new techniques 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 ¡100¿ rotation axes have higher energies and lower mobilities than ¡111¿ boundaries, for example. Annealing of the foil to develop the columnar structure reveals a progressive strengthening of the cube texture component, 001¡100¿. Treating 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-9632556.

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. Dregia 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 misorientation of the boundary. 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 ansotropy 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. Demirel, A.P. Kuprat[1], N.N. Carlson[2], D.C. George[1], G.K. Straub[1], A.D. Rollett, Carnegie Mellon University, Department of MS&E, PA. [1]Theoretical Division, Los Alamos National Laboratory, NM. [2]Computational 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=mk) 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:
1. A. Kuprat, "Modeling Microstructure Evolution using Gradient-Weighted Moving Finite Elements", LA-UR-98-4879, SIAM J. Sci. Comp., (1999).
2. Galen K. Straub, Denise C. George, Andrew P. Kuprat "Materials Microstructural Evolution in 3D Surface Front-Tracking Computer Simulations" LA-UR-00-1. Theoretical Division Self-Assessment Special Feature, (2000).
3. B.L. Adams, D. Kinderlehrer, W.W. Mullins, A.D. Rollett, S. Ta'asan, "Extracting the Relative Grain boundary Free Energy and Mobility function from the Geometry of Microstructures," Scripta Materialia, vol. 38, pg 531- 536 (1998).

11:45 AM Y1.9
PHASE-FIELD MODEL OF CRYSTAL GRAINS. Alexander E. Lobkovsky, 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 misorinetaion. We calculate the rate of rotation of a grain in the sharp interface limit and find that it depends sensitively on the choice of the model.

SESSION Y2: INTERFACE MOTION II – MICROMECHANISMS
Chairs: Anthony D. Rollett and Mark Aindow
Monday Afternoon, November 27, 2000
Independence E (Sheraton)

1:30 PM *Y2.1
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 attractive 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. Alessandra Satta and Luciano Colombo, INFM and Dipartimento di Fisica, Universita di Cagliari, Cagliari, ITALY; Fabrizio Cleri, ENEA, Divisione Materiali, Centro Ricerche Casaccia, and INFM, 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-twin 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-traction border conditions were performed on several 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 {it only 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 switching (in the Ashby-Verrall sense) and grain-disappearance events, respectively. We present preliminary results of the atomic-scale modelling of both classes of topological events and discuss the connection between atomistic and mesoscopic modelling of microstructural evolution. Work funded in part by the INFM-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. Haslam, S.R. Phillpot, D. Wolf and D. Moldovan, 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 a columnar grain structure. The conventional picture of grain growth is that the process is governed by curvature-driven grain-boundary (GB) migration. However, in our simulations grain rotations, leading to the coalescence of neighboring grains, play 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. Phillipp, 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 technique [1]. Twist and general GBs in addition to [110] and [001] tilt GBs could thus be prepared for HREM observation. Hence, for the first time it was possible to observe the atomic-scale motion of high-angle twist and GBs with finite twist and tilt components. Movement of GBs can proceed via thermal activation and with the aid 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 defect diffusion, dislocation glide, 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 sigma = 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 experiment, however 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 (001) grains provides a driving force for migration of twist and general GBs and the GB typically moves by the propagation of atomic-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 atomic-scale GB migration mechanisms and are consistent with theoretical considerations and molecular dynamics modeling studies of grain boundary migration in the literature. [1] K.L. Merkle 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 I
Chairs: Anthony D. Rollett and Mark Aindow
Monday Afternoon, November 27, 2000
Independence E (Sheraton)

3:30 PM *Y3.1
ANISOTROPIC GRAIN BOUNDARY PROPERTIES FROM ATOMISTIC CALCULATIONS. David J. Srolovitz, Moneesh Upmanyu, 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 mechanism. First, we present recent molecular dynamics simulation results on boundary mobility as a function of misorientation and temperature. The resultant 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 available. 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 foundary 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. Hamilton, Istvan Daruka, 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 Hsieh and Balluffi* shows a reversible de-faceting transition of incoherent twin boundaries in an aluminum thin film at about 400K. We initially modeled this transition using molecular dynamics and learned that the grain boundary 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 two-dimensional lattice model incorporating both the topology of the boundary and the energy associated with the excitation. Using a Metropolis Monte Carlo algorith we showed that 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. * T.E.Hsieh and R.W.Balluffi,"Observations of Roughening/Defaceting Phase Transitions in Grain Boundaries", Acta. metall. Vol. 37, 2133 (1989).

4:30 PM Y3.3
A NEW CONTINUUM SCALAR MODEL OF FACETS. Tinghui Xin, Harris Wong, 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 interfacial profile. This approach works fine if the surface energy anisotropy is weak and the interfacial profile is smooth. However, when the anisotropy increases, the surface profile starts to intercept 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. Lucadamo, 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 junctions between adjacent facets, we are investigating interfacial dynamics in the FCC Σ=3 system. [111] oriented Au films consisting 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
Chairs: Michael Zaiser and Michael V. Glazov
Tuesday Morning, November 28, 2000
Independence E (Sheraton)

8:30 AM *Y4.1
PHASE FIELD MICROELASTICITY APPROACH IN MODELING MICROSTRUCTURE EVOLUTION. A.G. Khachaturyan, Y.M. Jin, Rutgers Univ, Dept of Ceramic and Materials Engineering, Piscataway, NJ; Y.U. Wang, Rutgers Univ, Dept of Mechanical and Aerospace Engineering, Piscataway, NJ; A. Artemev, 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 Microelasticity theory proposed by one of the authors years ago. Being incorporated in the Phase Field formalism, the Phase Field Microelasticity theory provides the computational model, which makes it possible to realistically simulate 3-dimensional simulations of mesoscopic microstructures in coherent multiphase and multidomain systems during decomposition, ordering and martensitic transformation in single crystals and polycrystals (with and without crystal lattice defects). 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 (macroscopic strain, magnetization, polarization) to structural changes caused by the applied external fields (stress, magnetic field, electric fields).Using the Phase Field Microelasticity 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 automatically takes into account the strain-induced long-range interaction between 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 a

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 MS&E, University Park, PA.

A diffuse-interface field model is proposed for describing diffusional processes in coherent systems with arbitrary microstructures and arbitrary spatial distribution of structural defects such as dislocations, grain boundaries, cracks, and inclusions. It takes into account the effect of both the coherency 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 slip bands, and crack-like defects are considered. It is shown that coherent nucleation may become barrierless under the influence of the local elastic field of structural defects.

9:30 AM Y4.3
MICROSTRUCTURAL DEVELOPMENT UNDER NON-ISO-THERMAL CONDITIONS USING THE PHASE FIELD METHOD. J.P. Simmons, AFRL/MLLM, Wright-Patterson AFB, Dayton, OH; S. Chen, Y. Wang, The Ohio State University, Columbus, OH.

Processing 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 particles, shows much promise in these systems. However, 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 include non-isothermal processes such as continuous cooling. Results of non-isothermal processing on transformation behavior and microstructural development will be given.

9:45 AM Y4.4
PHASE FIELD MICROELASTICITY MODEL IN STUDY OF THE INFLUENCES OF DEFECTS ON MARTENSITIC MICRO-STRUCTURE EVOLUTION. Yongmei M. Jin, Rutgers Univ, Dept of Ceramics and Materials Engineering, Piscataway, NJ; Andrei Artemev, Carleton Univ, Dept of Mechanical and Aerospace Engineering, Ottawa, CANADA; Armen G. Khachaturyan, Rutgers Univ, Dept of Ceramics and Materials Engineering, Piscataway, NJ.

The Phase Field Microelasticity (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 *a priori* 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 mesoscopic morphology under various undercooling 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 MACRO-SCOPIC 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. Ni_3Al) whereas others show a monotonic decrease with increasing temperatures (e.g. Pt_3Al and doped Al_3Ti, although they crystallize in the same structure as Ni_3Al). It is demonstrated by a multiscale analysis that these differences can be traced back to differences in the electronic structure. Starting point is a phenomenological model for the nonmonotonic yield stress, the Kear-Wilsdorf model, which relates the macroscopic plastic behaviour to the structure of the individual superdislocations. The atomistic structure of the dissociated superdislocations is determined by the generalized Peierls model which is a combination of anisotropic elasticity theory and discrete-lattice theory. The atomistic input information required for this model is provided by the ab-initio density functional electron theory. It is shown that 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 structures of the superdislocations as 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 two Shockley partials which controls the rate of cross-slip between crystallographic planes and hence the rate of dislocation self-trapping is calculated for Ni_3Al.

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

The McCormick model for dynamic strain ageing is explored using modern methods of nonlinear dynamics. The quintic (fifth-order) 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 linear stability analysis and to probe the actual instability 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 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 strongly 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 6xxx series aluminum alloy and yielded promising results in terms of predicting the Ludering 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. Roytburd, Department of Materials and Nuclear Engineering, University of Maryland, College Park, MD.

The effect of the relaxation on microstructure, thermodynamics and kinetics of diffusionless transformations is considered. Internal stresses in a transforming crystal stimulate formation and movement of defects, especially dislocations. Nets of dislocations emerge on 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 to a great extent define the mobility of interphase interfaces. 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, Rensselaer Polytechnic Institute, Troy, NY; S.P. Marsh, Physical Metallurgy Branch, Naval Research Laboratory, Washington, DC.

Phase coarsening plays a fundamental role in late stages of microstructure evolution. Numerous processes, such as casting, sintering, precipitate aging and industrial crystallization depend on phase coarsening. A continuum theory of phase coarsening employing global constraints was developed several years ago on the basis of LaPlacian diffusion and screening to account for the effect of finite volume fraction on coarsening rates. 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 Marqusee 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 locale noise is found to broaden the PSD and eliminate the need for the well-known LSW stability criterion based on mass conservation. Progress in applying stochastics and diffusion screening in late-stage phase coarsening and microstructure evolution theory will be discussed.

11:45 AM Y4.9
PHASE FIELD METHODS AND DISLOCATIONS. A. Finel, Lab d'Etude des Microstructures (ONERA-CNRS), Cedex, FRANCE; D. Rodney, LEM (ONERA-CNRS), Cedex, 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 that we can incorporate the dynamics of the disclocations into the same formalism. This extends the applicability of the Phase Field methods to the new area of plastic properties of crystalline solids.

SESSION Y5: SOLIDIFICATION
Chairs: Mark D. Asta and Anthony D. Rollett
Tuesday Afternoon, November 28, 2000
Independence E (Sheraton)

1:30 PM *Y5.1
BRIDGING LENGTH SCALES IN SOLIDIFICATION BY LINKING ATOMISTIC AND PHASE-FIELD SIMULATIONS. Jean Bragard, Alain Karma, Physics Dept, Northeastern Univ, Boston, MA; Mathis Plapp, Laboratoire de Physique de la Matière Condensée, CNRS/Ecole Polytechnique, Palaiseau, FRANCE.

A Computational Materials Science Network (CMSN) was recently created that brings together atomistic and continuum scale simulations in order to significantly enhance the predictive capabilities of current 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 input into phase-field models to make quantitative predictions that can be compared to experiments. Simulation results will be presented that shed new light on the origin of a widely observed, albeit so far unexplained, growth morphology transition in highly undercooled metallic melts.

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

The microscopic solvability 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/m^2 is found for the interfacial energy, in good agreement with empirical estimates, and an anisotropy between the 100 and 110 crystal faces of 3.7% 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 = 45, 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. Jamie R. Morris, Zhong-Yi Lu, 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 SOLID-LIQUID INTERFACES IN Cu-Ni ALLOYS. Harish Ramalingam and Mark Asta, Northwestern University, Dept. of MS&E, 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 Cu-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 variations in composition, density and energy normal to the interface. From these results we back out equilibrium solidus and liquidus boundaries predicted by the embedded-atom-method interatomic potentials used in our simulations. The equilibrated structures obtained from Monte-Carlo provide the starting point for molecular-dynamics simulation studies of the equilibrium dynamical properties of solid-liquid interfaces in Cu-Ni alloys. This work is supported by the Department of Energy under contract number DE-AC04-94AL85000.

3:30 PM *Y5.5
DENDRITIC GROWTH DYNAMICS: STEADY AND OSCILLATORY STATES. M.E. Glicksman, J.C. LaCombe, M.B. Koss, A.O. Lupulescu, C. Giummarra, J.E. Frei, MS&E, Rensselaer Polytechnic Institute, Troy, NY.

Microgravity dendritic growth experiments, conducted aboard the space shuttle Columbia (STS-87) in November/December 1997, are analyzed and discussed. In-situ video images now 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 transient features 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 as 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 Greens 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 growths 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, Foundry Institute, Aachen, GERMANY.

Semi-solid metal alloys exhibit a shear-rate history-dependent flow

response during injection into a die. The increasing interest from the thixo-casting industry makes the understanding of the flow behavior of the thixotropic metal alloys necessary. The viscosity of liquid materials is frequently measured with a capillary viscometer. This technique was used to investigate the rheology of semi-solid 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 two 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 SOLIDIFICATION. Vadim S. Zolotorevskij, 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 AI-Cu-Mg, AI-Zn-Mg and AI-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^{-1}-10^{2} K/s. It was determined that at Vc$\leq$20 K/c (Al) most of the alloys had a cellular dislocation structure. In the alloys with 8-14 at. % Mg, a polygonal (subgranular) structure forms, whereas in the alloys with lesser Mg content and in the ternary Al-Zn-Mg alloys a mixed (cellular - subgranular) type of structure forms. The total dislocation density in all the alloys usually was of one order of magnitude - 10^{9} cm^{-2}, sometimes - 10^{8} (at small Vc) or 10^{10} cm^{-2} (at maximum Vc and subgranular structure). The difference between dislocation densities in the cast alloys has a certain 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. In alloys with a distribution coefficient k¡1, the dislocation density attains the maximum value, while the sizes of subgrains and dislocation cells are minimal. It was shown that the contributions of concentration, contraction and thermal stresses in the dislocation structure formation of (Al) are not significant. Just as dislocation densities which are calculated from the dendrite cells size and average angle of their misorientation are close to those experimentally determined. On that basis it was supposed that the main part of dislocations in castings forms as a result of growth of dendrite branches and their coalescence.

4:45 PM Y5.8
EFFECT OF ULTRASONIC (CAVITATION) TREATMENT OF THE MELT ON THE MICROSTRUCTURE EVOLUTION DURING SOLIDIFICATION OF ALUMINUM ALLOY. Georgy Eskin, All-Russia Institute of Light Alloys, Moscow, RUSSIA.

During past 30 years, All-Russia 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 aoustic cavitation in the formation, pulsation and coagulation of fine hydrogen bubbles. Such bubbles are easily formed at the surface of nonwettable disperse solid inclusions ("plankton") 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 during degassing, cleaning and solidification.
Because of nonlinear pulsations induced by ultrasound, cavitation bubbles start to pulsate and subsequently either transform into macroscopic gaseous 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 sonocapillary effect and the wetting of fine nonmetallic particles in the melt.
The multiplication of solidifiation nuclei upon cavitation melt treatment changes the evolution of structure during solidification. With respect to the intensity of cavitation process in the melt upon ultrasonic treatment, it is possible to form the ultimately refined, nondendritic grain 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 the production of large-scale, crack-free ingots from commercial structural aluminimum 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 nondentic strucure facilitates semi-solid processing of alloys.
Reference:
G.I. Eskin, Ultrasonic Treatment of Light Alloy Melts, Gordon and Breach, Amsterdam, 1998.

SESSION Y6/Z5: JOINT SESSION
STRAIN LOCALIZATION AND DISLOCATION PATTERNING
Chairs: Michael Zaiser and Elias C. Aifantis
Wednesday Morning, November 29, 2000
Independence (Sheraton)

8:30 AM *Y6.1/Z5.1
SPATIAL DISTRIBUTIONS OF DISLOCATION STRUCTURES FROM MILLIMETERS TO NANOMETERS. 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 fcc metals is a cell block. A cell block is composed of cell block boundaries (flat extended geometrically necessary boundaries, GNBs) and cell boundaries (short incidental 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 neighbor. This difference is in accord with the difference 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 roughly from 10x100x100 micrometers to 10x100x100 nanometers. Misorientation angles can range from 1 to 62.8 degrees. Thus the cell blocks accumulate a record of the slip pattern. Mapping the distribution of the cell block parameters, either 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 friction, sample grips, and test platens. This is illustrated by comparisons dislocation structures that form in single crystals, bicrystals and polycrystals as a function of strain.
This work was supported by the U.S. DOE Office of Basic Energy Sciences, Division of Materials Sciences under contract no. DE-AC04-94AL85000.

9:00 AM *Y6.2/Z5.2
DEVELOPMENT, SCALING AND EVOLUTION OF DISLOCATION CELL SUBSTRUCTURES. Elizabeth A. Holm, Sandia National Laboratories, Albuquerque, NM; Richard A. LeSar, Los Alamos National Laboratory, Los Alamos, NM; Mark A. Miodownik, Dept. of Mechanical Engineering, University College Dublin, IRELAND.

The development of a dislocation cell substructure has been observed in a wide variety of plastically 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 entropy (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 cellular automaton model for microstructural evolution, and cell size scaling is observed. Evolution of the cell substructure occurs by uniform recovery, with self-similar cell size and misorientation distributions characterized by a continuously increasing average cell

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. Mark A. Miodownik, 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 a non-equilibrium state at the beginning of the simulation. As a result of dislocation 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 abnormal cells do not need to be artificially introduced but occur naturally as outliers in 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.B. 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 rotator 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 close analogs of screw dislocations, and the applied twist rate is analogous to an applied 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 both temperature and strain rate. Both channel spacing and overall defect density obey scaling relationships 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, at temperatures well below the Kosterlitz-Thouless 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 rotator 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 Khantha-Pope-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 MODELING. Peter Hähner, 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 quasi-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 those 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 those 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 dislocations distributions corresponding to hierarchically organized dislocation cell structures are obtained, while in the latter case a decomposition into dislocation-rich walls or veins 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 fcc metals. The close agreement points at the importance of collective dislocation effects in the self-organization of those structures.

11:00 AM Y6.6/Z5.6
STATISTICAL PROPERTIES OF DISLOCATION ASSEMBLIES. I. Groma, Eötvös University Budapest, Department of General Physics, Budapest, HUNGARY.

It is well known that during the plastic deformation of crystalline materials 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 organizatory 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 to overcome this 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 the behavior of a system of straight parallel dislocations is investigated. It is found by numerical simulation that the internal stress τ 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 $1/\tau^3$.

11:15 AM Y6.7/Z5.7
DISLOCATION MULTIPLICATION 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 crystals and the associated yield-point, several questions remain open. A study of this phenomenon is underway on Ge single crystals oriented in single glide. Monotonous compression tests are performed together with transients (relaxation and creep tests) at various temperatures (650 - 850 K) and strain-rates (10^{-5} to $4.10^{-4}s^{-1}$). Dislocation structures are observed in the transmissioon 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 covalent material (Si) performed by Moulin, Condat, Kubin (Acta Mater. 1999).

11:30 AM Y6.8/Z5.8
SIMULATION OF DISLOCATION CELL STRUCTURES. Benoit Devincre, Diego Gomez-Garcia, Ladislas P. Kubin, LEM, CNRS-ONERA, Chatillon, 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 multislip conditions. In BCC crystals cell structures are also formed in conditions of stain and temperature such that the interactions between dislocations prevails

over the lattice friction. The objectives of dislocation dynamics simulations in this domain are to reproduce dislocation cell formation, define the leading mechanisms that contribute to it and, possibly, 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 multislip 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 mechanisms 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 locks, serve as anchoring points for the formation of dislocation cells. Once the latter are formed, a pattern of long-range stresses is established that enhances their further development. Attempts to investigate the origin of the similitude principle are discussed with the help of a 2.5-D simulation that mimics in 2-D the three-dimensional mechanisms described above.

11:45 AM Y6.9/Z5.9
STRAIN GRADIENTS AND PATTERNING OF PLASTIC FLOW. John L. Bassani, 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 slips that contribute significantly to overall hardening behavior also play an important role in the nucleation and stabilization of such localized modes of deformation. These secondary slips can also control patterning, e.g. thickness and spacing of coarse slip bands, through the effects of lattice incompatibility. 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 enters the instantaneous hardening relations. As a result, the classical bifurcation 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
Chairs: Michael V. Glazov and Elizabeth A. Holm
Wednesday Afternoon, November 29, 2000
Independence E (Sheraton)

1:30 PM *Y7.1
PHENOMENOLOGICAL AND EXPERIMENTAL DEVELOPMENT IN QUANTIFYING PLASTIC DEFORMATION. Vivek Sample, 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 history.
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 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, INFM, Universitá La Sapienza, 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 yield stress. Numerical simulations of a discretized version of the equation confirm these results 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. Fabrizio Cleri and Gregorio D'Agostino, ENEA, Divisione Materiali, Centro Ricerche Casaccia, and INFM, 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. Cleri, Physica A {bf 282, 339 (2000)). 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 the 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 in two dimensions of point-like, interacting dislocations whose density and position affects grain–boundary migration. Work funded in part by the INFM-Forum Project MUSIC "Multiscale Simulation of Complex Materials" and the ENEA Project FOTO "Laser-induced recrystallization of amorphous silicon".

2:30 PM Y7.4
A GENERAL MONTE CARLO APPROACH FOR MODELING 3-D DISLOCATION MICROSTRUCTURES. Sriram Swaminarayan 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 the 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 different 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 Dolgert, 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 deforming materials. We have used large-scale molecular dynamics simulations on parallel computers to study the interactions of crystal defects in metals. 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 vacancies, and a low density of dislocations in the 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 foil 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 annihilation 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 strained bicrystal. The 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 causes the grain boundary to emit new dislocations 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 Heinisch, Jr., Rick Kurtz, Pacific Northwest National Laboratory, Richland, WA; Dick Hoagland, Los Alamos National Laboratory, Los Alamos, NM.

Atomistic 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 (dilatant center) that falls off as $1/r^2$. 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 not coincident with the dislocation origin for the edge dislocation but was coincident for the screw. The origin of the dipole was found to be in the compressive region of the edge dislocation, as expected. 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 in terms of its area of expansion, δA, be constant in the volume of the model evaluated on all contours that included the defect. The force between two dislocations within a distance of 10b was calculated using the Volterra plus dipole field and compared to standard elastic calculations that ignore the core field. The results are discussed in the context of discrete dislocation dynamics and dislocation-dislocation interactions.

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

We use atomistic simulations to characterize the dislocation activity in the plastic zone surrounding a void growing under tensile loading. Multi-million atom molecular dynamics simulations have been run on a systems initially consisting of a periodic box, filled with atoms in a single crystalline or polycrystalline array. [1] A dilatational strain is applied that induces void growth, which is accommodated by dislocation generation in the volume immediately surrounding the void. We have studied the resulting dislocation systems in FCC 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 play an important role in the ensuing evolution of the void. [2] The junctions allow the formation of a generalization of prismatic dislocation loops, which facilitate outward material transport and accommodate the growing void. We further identify the character of the most numerous dislocations and their associated glide planes. The results are in agreement with experiment when account is taken of the strain rate difference. Acknowledgement: This work was performed under the auspices of the US Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48. [1] J. Belak, "On the nucleation and growth of voids at high strain-rates," J. Comp.-Aided Mater. Design 5, 193 (1998). [2] J. Belak and R. Minich, "Simulation of void growth at high strain-rate," Proc. Symposium Fracture - Theory, Modelling and Experiment, Boston, MA, USA, 30 Nov.-3 Dec. 1998, (Mater. Res. Soc., Warrendale, PA, USA, 1999), pp. 257-61.

4:15 PM Y7.9
EFFECT OF BOUNDARY CONDITIONS IN ATOMISTIC SIMULATIONS OF VOID GROWTH. R.R. Settgast, Dept of Civil & Environmental Engineering, Univ of California-Davis, Davis, CA; B.P. Somerday and M.F. Horstemeyer, Sandia National Laboratories, Livermore, CA; M.I. Baskes, 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 related to void size, void spacing, and lattice (grain) 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-displacement versus fixed-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 loading rate is examined by conducting quasi-static energy minimizations as well as finite-rate molecular dynamics simulations. The lattices of interest are nickel containing initial one-void and two-void configurations.

SESSION Y8: POSTER SESSION
Chairs: Douglas L. Medlin, Michael Zaiser, Mark Aindow, Michael V. Glazov, Anthony D. Rollett and Mark D. Asta
Wednesday Evening, November 29, 2000
8:00 PM
Exhibition Hall D (Hynes)

Y8.1
EVOLUTION OF NANOSTRUCTURE OF FeNi(Ti/Cr)N ALLOYS DURING PHASE CYCLING. N.G. Chechenin, P.M. Bronsveld, A. Chezan, C.B. Craus, D.O. Boerma, J. Th. M.de Hosson and L. Niesen, Univ. of Groningen, Materials Science Centre, THE NETHERLANDS.

A possibility to manipulate the microstructure of cold rolled (down to less than 1% of the initial thickness) $Fe_{94}Ni_4Ti_2$ and $Fe_{93}Ni_4Cr_3$ foils via inter-phase cycling by nitriding and de-nitriding is investigated. As determined by light microscopy, XRD and TEM, at this severe deformation the grains in the as-rolled samples had a complicated uneven shape: they spread out to a size between 1 and 20 μm in the plane parallel to the surface and are squeezed to about 100-500 nm in the perpendicular direction. Also the grains had a complicated internal nanostructure due to a dislocation network, forming cells of 10 nm size. This cells or subgrains were coherent, producing an overall (001)[110] texture with some admixture of {111} and {311} textures. We observed, that the $\alpha \Longleftrightarrow \gamma$' transformation was accompained with some dispersion of orientation of subgrains, while the overall coherency between secondary and parent phases remained. Similar processes are also valid for the reverse transformation $\gamma' \Longrightarrow \alpha$, thus explaining the persistent texture in cycled samples. However, due to the misorientation of the subgrains, the texture in the cycled samples will be less pronounced. It was observed that the lamellar structure present in the γ' phase is coarsening with the number of cycles. A reduction of the texture was obtained in the $\epsilon \Longleftrightarrow \alpha$- cycling, when nanosized grains with a new orientation appear in XRD scans. It was found that the phase transition to γ' or ϵ was slowing down with the number of cycles. A model to explane this observation will be presented.

Y8.2
INFLUENCE OF MICROSTRUCTURE OF PRECURSOR DERIVED Si-C-N CERAMICS ON THEIR MECHANICAL PROPERTIES. Arndt Bauer, André Zimmermann, Joachim Bill, Fritz Aldinger, Max-Planck-Institut für Metallforschung and Institut für

Nichtmetallische Anorganische Materialien, Universität Stuttgart, Pulvermetallurgisches Laboratorium, Stuttgart, GERMANY.

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 mechanical creep resistance of Si-C-N 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-C-N 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 a 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 R-curve measurements with DCB-speciments.

Y8.3
EVOLUTION OF MICROSTRUCTURE AND DEFECT STRUCTURE DURING NUCLEATION AND GROWTH OF THE $L1_0$ PHASE IN MANGANESE-ALUMINUM. Cagatay Yanar, Jorg M.K. Wiezorek, William A. Soffa, Dept. of MS&E, University of Pittsburgh, Pittsburgh, PA; Velimir Radmilovic, Department of Physical Metallurgy, University of Belgrade, Belgrade, SERBIA.

Manganese-aluminum alloys in the vicinity of the equiatomic composition exhibit an attractive combination of magnetic properties for application in various devices including thin films. These technical magnetic properties derive from the formation of a metastable $L1_0$ intermetallic phase (τ - MnAl) characterized by a high, uniaxial magnetocrystalline anisotropy with an easy "c-axis." Carbon is generally added to stabilize the tetragonal τ - MnAl 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 τ - phase ($L1_0$) within the parent high-temperature epsilon-phase (hcp). 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 polytwinned microstructures and the profusion of planar defects characteristic of the MnAl-base ferromagnets.

Y8.4
INFLUENCE OF DISLOCATIONS ON DEUTERIDE FORMATION IN SINGLE CRYSTAL PALLADIUM. W.C. Chen and Brent J. Heuser, University of Illinois, Dept. Nuclear, Plasma, and Radiological Engineering, Urbana, IL.

The effect of dislocations on deuteride formation in the Pd-D system has been investigated with small-angle neutron scattering (SANS) and in situ transmission electron microscopy (TEM). SANS is extremely sensitive to bulk deuteride formation (use of deuterium results in greater foreground and lower background signals) in metals, 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 hydride miscibility gap. The characteristic response from small, 20-30 Angstrom thick, plate-like particles has been observed in the SANS measurement of both sample types. We believe these small plates are coherent with the host Pd lattice and act as precursors to the formation of much larger, tens-of-microns thick incoherent plate-like particles. 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 minimization of strain energy along the elastically-soft ¡100¿ direction. We believe the ¡110¿ habit plane is the result of the dislocation substructure influencing the precipitation process. This hypothesis is support by SANS 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 observations 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 1.6%Ce, 1.6%Ni, 4.9%Ge, 22.8%Co, and 69.1%Sb alloy, both isolated dislocation dipoles and arrays of dislocation dipoles are observed. Mechanisms for reducing the strain energy of the expected large Burgers vector, approximately 8Å, are analyzed, including the possibility of segregation of alloying elements along the dislocation cores.

Y8.6
DISLOCATION DIPOLE CONFIGURATION IN GaInP-GaAs HETEROSTRUCTURES. Y.Q. Wang and Z.L. Wang, School of MS&E, Georgia Institute of Technology, Atlanta, GA; T. Brown, A. Brown and G. May, Department of Electrical Engineering, Georgia Institute of Technology, Atlanta, GA.

Misfit dislocation dipoles, in which two parallel dislocations are separated by about 3.5nm, have been observed in the solid source MBE GaInP lattice-matched to GaAs heterostructures (mismatch strain: 0.093%). The dislocations are not exactly located at the interface. They are actually distributed in a zone of 3 - 5 nm wide in the GaInP 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 positions, 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 GaInP epilayer.

Y8.7
INFLUENCE OF ANTIMONY DOPING ON NANOSCALE ARSENIC CLUSTERS AND DISLOCATION LOOPS IN LOW-TEMPERATURE GROWN GALLIUM ARSENIDE FILMS. V.V. Chaldyshev, N.A. Bert, A.E. Romanov, A.A. Suvorova, Ioffe Institute, St. Petersburg, RUSSIA; A.L. Kolesnikova, Institute for Problems of Mechanical Engineering, St. Petersburg, RUSSIA; V.V. Preobrazhenskii, M.A. Putyato, B.R. Semyagin, Institute of Semiconductor Physics, Novosibirsk, RUSSIA; P. Werner, Max-Plank Institut für Mikrostrukturphysik, Halle/Saale, GERMANY.

Gallium arsenide grown by molecular-beam epitaxy (MBE) at low temperature (LT) has attracted much attention due to ultra-short carrier lifetime and excellent electrical insulation properties. This material contains a very high arsenic excess which precipitates upon post-growth anneals, so that a system of nanoscale As 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-contained structures without extended defects, such as dislocations, stacking faults, etc. On the other hand, 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 strain was reached 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 (001) plains. The system of a nanoscale cluster with anisotropic 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 (001). This approach, which we call patterned heteroepitaxial processing (PHP), involves post-growth patterning and thermal annealing. Whereas pregrowth substrate patterning 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 (001) were grown to thicknesses of 2000 - 6000 $\approx$ by photoassisted metalorganic vapor phase epitaxy (MOVPE). Following growth, layers were patterned by photolithography and then annealed at elevated temperature under flowing hydrogen. Threading dislocation densities were determined using a bromine/methanol etch followed by microscopic evaluation of the resulting etch pit densities. We found that as-grown layers contained more than 10^7 cm^{-2} threading dislocations. The complete removal of threading dislocations was accomplished by patterning to 70 μm by 70 μm square regions followed by thermal annealing for 30 minutes at temperatures greater than 500°C. Neither post-growth annealing alone nor post-growth patterning alone had a significant effect. The effectiveness of this approach diminishes significantly below 500°C so that annealing at 400°C produces no measurable effect. Partial removal of dislocations was observed at temperatures between 400°C and 500°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.

Y8.9
DISLOCATION DENSITY REDUCTION VIA LATERAL EPITAXIAL OVERGROWTH IN GaSb GROWN ON PATTERNED GaAs SUBSTRATES. S.S. Yi, D.M. Hansen, B.E. Hawkins, T.F. Kuech, Dept of Chemical Engineering, Univ of Wisconsin, Madison, WI; C.K. Inoki, D.L. Harris, T.S. Kuan, Dept of Physics, Univ at Albany, State Univ of New York, Albany, NY.

Lateral epitaxial overgrowth (LEO) refers to spatially-controlled growth of an epitaxial 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-lived 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, GaAs 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 $\sim 10^{10}/cm^2$. 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 metalorganic 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 $10^6/cm^2$. Local stress simulation indicates that the local stress gradient near a small opening is effective in bending and confining dislocations to within ~ 2 μm from the growth window, resulting in significant dislocation density reduction.

Y8.10
INTERFACIAL REACTIONS IN SOLDER/METALLIZATION DIFFUSION COUPLES IN LIQUID AND SOLID STATE. A. Zribi, R.R. Chromik, L. Zavalij, E.J. Cotts, State University of New York in Binghamton, Physics Department, NY.

As length scales decrease in electronics packages, kinetic considerations have come to dominate solder alloy formation processes. Phase selection at solder/metal interfaces is determined by which phase grows the fastest, i.e. by kinetics, rather than by energetics. Diffusion rates of metal atoms such as Cu, Au or Ni in Sn are orders of magnitude higher than those of Sn in standard metallization constituents. In fact, the most Sn-rich phase (such as $PdSn_4$, or Cu_6Sn_5) in a Sn-metal system is generally found to form first in conventional PbSn solder/metal diffusion couples. With the advent of Pb-free solders, solder/metal systems have become more complex. While Pb is removed from these solders, relatively small amounts (a few atomic percent) of metal atoms such as Ag or Cu are added to Sn to lower melting points of the solders and improve their mechanical properties. Moreover some metallizations are coated with a layer of Au which dissolves rapidly into solder upon melting. Thus a small atomic percentage of metal atoms such as Cu or Ni can be found in a Sn matrix in Pb-free solders. Because these species diffuse at high rates in Sn, investigation of interfacial growth processes in Pb-free solder/metallization couples must consider growth of alloys with relatively high concentrations of these elements. In fact, we observe a number of interface growth processes determined by the ternary addition of one of these constituents, e.g. the formation of $(AuNi)Sn_4$ at Ni/solder interfaces upon thermal aging, or the formation of $(CuNi)_6Sn_5$ at Ni/solder interfaces. We present results of our observations of these growth processes. We consider the impact of defect structures of the growing solder alloys in determining growth rates, and thus phase selection. We attempt to characterize the kinetics of these processes with simple models, including diffusion rates in both solid and liquid states.

Y8.11
MODELING OF PHASE TRANSFORMATION DURING HOMOGENIZATION OF TERNARY ALUMINUM ALLOYS. Th. Hofmeister, K. Greven, A. Ludwig, P.R. Sahm, RWTH-Aachen, Foundry Institute, Aachen, GERMANY.

The microstructure determines for the most part mechanical properties of castings. This is the case especially with age-hardening aluminum alloys. To predict the phase transformation in cast parts during and after solidification a sophisticated approach to a coupled modeling of various simulation phenomena is presented. This approach couples a diffusion equation solver which considers the online estimation of thermodynamic equilibria 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 back diffusion, 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 areas 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. Olof C. Hellman and David N. Seidman, Dept. of MS&E, 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 potentials 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 stability of different grain 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 energies of different boundaries. This research is supported by the National Science Foundation, Division of Materials Research, Grant DMR-972896, Bruce MacDonald, Grant Officer.

Y8.13
THE EFFECTS OF A NEW GRAIN BOUNDARY PHASE IN Ni-Al ALLOY. Y.L Chiu, A.H.W. Ngan, 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 microscope (CTEM). This phase is identified to be of C_6Cr_23 type structure with unit lattice parameter of 10.48 angstroms, which is approximately three times that of Ni_3Al 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 post-mortem specimens which have been carefully deformed with nano-indentor after jet-polishing. The formation mechanism of the precipitate during the heat-treatment process and correlation with the significantly improved ductility of the boron-doped alloy will also be discussed.

Y8.14
INTERFACE STRUCTURE IN FERRITIC/AUSTENITIC STAINLESS STEEL BICRYSTALS. A. Taisne, B. Décamps, Laboratoire de Chimie Métallurgique des Terres Rares, UPR 209 du

CNRS, Groupe des Laboratoires de Vitry-Thiais, Thiais Cedex, FRANCE; L. Priester, Laboratoire d'Etudes des Matériaux Hors Equilibre, UMR 8647, Université Paris-Sud, Orsay Cedex, FRANCE.

Interactions between lattice dislocations and interfaces play an important role in the plastic deformation of materials. Stress concentrations may build-up and eventually relax under the mechanical solicitation depending on the temperature. The different processes have been investigated in grain boundaries in different materials but there are very few studies of these processes for interphase interfaces. Most often, only the dislocation configurations at vicinity of the interface in the neighbouring crystals have been analysed but no information on the phenomena within the interface have been until now pointed out. The aim of this work is to study the elementary mechanisms occurring at the ferrite/ austenite interfaces in duplex stainless steels which have been deformed by fatigue. The compositions of the two phases are : for the ferrite Fe-30Cr and for the austenite Fe15Cr15Ni. The experiments are performed on steel bicrystals obtained by diffusion bonding which display different orientation relationships and which are plastically compatible or not. The final goal is to establish a correlation with the macroscopic behaviour (1). A combination of two transmission electron microscopy techniques, conventional bright/dark field and weak beam, assisted by image contrast simulation is used to study the bicrystal microstructure. The results include the following informations: Accurate determination of the $\alpha/\ \gamma$ interface crystallography (misorientation between phases and interface plane orientation). Characterisation of dislocations (Burgers vector and dislocation line) and activated slip system in each phase. Fine analysis of interfacial dislocations. On the basis of these analyses, elementary mechanisms of stress accommodation at $\alpha/\ \gamma$ interfaces are discussed. (1) Wada T. and Hashimoto S., Materials Science Forum, vols.294-296 (1999) 693.

Y8.15
Abstract Withdrawn.

Y8.16
GRAIN BOUNDARY STRUCTURE IN B2 Fe-Al ORDERED ALLOYS: AN ATOMIC-SCALE SIMULATION. R. Besson, C.S. Becquart, A. Legris, Laboratoire de Métallurgie Physique et de Génie des Matèriaux, C.N.R.S. U.M.R. 8517, Université des Sciences et Technologies de Lille, Bütiment C6, Villeneuve d'Ascq, FRANCE; J. Morillo, Structure des Systemes de Basse Dimensionnalite, CNRS/CEMES 29, Toulouse, FRANCE. On leave from Laboratoire des Solides Irradiés, Commissariat l'Energie Atomique, CNRS UMR 7246, Ecole Polytechnique, Palaiseau, FRANCE.

Given their high intrinsic properties, transition metal aluminides are considered as possible candidates in replacing alloys nowadays used in severe conditions. However, their industrial use is still delayed by their strong intergranular brittleness which is probably related to the atomic structure of grain boundaries. This point is particularly well tackled by atomistic simulations. In this work, we present results concerning the atomic structure of the (310)[001] symmetrical tilt grain boundary (GB) in B2 Fe-Al ordered alloys. The alloy is modeled using N-body empirical potentials and ab initio calculations based on the density functional theory. All low energy GB variants are found to be geometrically close to the usual symmetric and pseudosymmetric ones deduced from the coincidence site lattice (CSL) theory. However, strong chemical effects are found, that cannot be obtained by simple application of CSL theory. This shows that GB structures and therefore alloy mechanical properties may be strongly influenced by bulk composition. The validity of the independent point defect approximation, generally used to describe GB segregation, is also discussed.

Y8.17
STRUCTURE AND ENERGETICS OF LONG-PERIOD TILT GRAIN BOUNDARIES: AN EFFECTIVE HAMILTONIAN APPROACH. Dnyanesh Pawaskar[1], Ronald Miller[2], Rob Phillips[1]. [1]Div of Engr, Brown Univ, Providence, RI. [2]Dept of Mechanical Engr, Univ of Saskatchewan, Saskatoon, CANADA.

We have investigated the atomic-level structures of 44 <110> symmetric tilt grain boundaries in aluminum. The focus has been on examining the efficacy of the structural unit model in the context of very long period grain boundaries. Our studies, which have been carried out using two embedded-atom potentials, of both equilibrium as well as metastable structures of a number of boundaries reveal that the structural unit model must be supplemented with energetic considerations. An effective Hamiltonian is introduced to this end which computes the energy of a string of structural units constituting a grain boundary using two-body potentials between individual units. The potentials are calculated via a least-squares fit. Results with even 16 inputs are very encouraging and clearly demonstrate the effectiveness of this method, thus allowing for prediction of the structures of very long period boundaries.

Y8.18
UNDERSTANDING AND CONTROLLING INTRINSIC STRESSES CAUSED BY GRAIN BOUNDARY FORMATION IN POLY-CRYSTALLINE FILMS AND COATINGS. Brian W. Sheldon, Ashok Rajamani, Aaron Lau, Janet Rankin, J. Rod Beresford, Brown University, Division of Engineering, Providence, RI; Barbara L. Walden, Trinity College, Dept. of Physics, Hartford, CT.

A number of researchers have attributed large intrinsic tensile stresses which are created during film growth to grain boundary formation during the early stages of deposition. However, previous models of this phenomena do not provide accurate descriptions of stress evolution during growth. The tradeoff between elastic strain, surface, and grain boundary energies is complicated by microstructural effects such as surface roughness, grain size distributions, and the presence of different surface facets. We have developed models of growth and stress evolution due to island coalescence, using finite element methods and several approaches for describing kinetic processes. Results from these models will be compared to experiments with several different materials, including CVD diamond and epitaxial nitrides. In all of these cases, significant tensile stress evolves during the early stages of deposition, as islands coalescence to form a continuous film. Experimentally, large reductions in these intrinsic stresses were obtained by controlling the coalescence process. In particular, changes in the deposition chemistry during island coalescence can have a significant effect on the resultant intrinsic stress.

Y8.19
Transferred to Y1.8.

Y8.20
SIMULTANEOUS GRAIN BOUNDARY MIGRATION AND GRAIN ROTATION. Moneesh Upmanyu[1,2,3], David J. Srolovitz[2,3], W. Craig Carter[4] and James. A. Warren[5]. [1]Dept. of MS&E, University of Michigan, Ann Arbor, MI. [2]Dept. of Mechanical and Aerospace Engr., Princeton University, Princeton, NJ. [3]Princeton Materials Institute, Princeton, NJ. [4]Dept. of MS&E, MIT, Cambridge, MA. [5]Metallurgy Division, MS&E Laboratory, NIST, Gaithersburg, MD.

There are two distinct mechanisms by which grains can disappear during grain growth processes: namely, grain boundary migration and grain rotation. While the former is well known and clearly dominates at large grain sizes, there is an increasing body of evidence that suggests grain rotation may be important for small grains. We perform atomistic and phase field simulation that demonstrate that both processes occur simultaneously in small grains. Molecular dynamics simulations of a shrinking grain embedded within a single crystal were performed in two-dimensions with empirical potentials over a range of misorientations (including both low sigma and irrational boundaries). Both grain size and grain orientation were monitored as a function of time. The simulations show that for the range of initial misorientations simulated nearly all grains showed some degree of rotation while shrinking. In all cases, the grains rotated from their initial misorientation (between 10° and 30°) to a misorientation of ~21°, corresponding to a Σ=7 misorientation. While this misorientation corresponds to a cusp in the boundary energy/misorientation plot, so do the Σ=13 (28°) and 19 (13.17°) boundaries. Nonetheless, the shrinking grains rotate through these other low sigma misorientations. Preliminary analysis suggests that the grain rotation mechanism is associated with both diffusive effects and dislocation emission / absorption. A new phase field model that includes an accurate description of grain boundary anisotropy was applied to simulate grain shrinking, as in the atomistic simulations. The atomistic results are used to determine parameters in the phase field model. These simulations also show simultaneous grain boundary migration and grain rotation. Detailed comparisons between the atomistic and phase field results provide both validation for the phase field approach as well as a method for determining its limitations.

Y8.21
A SEMI-ATOMISTIC APPROACH TO OSTWALD RIPENING. Martin Schwind and John Agren, Dept. MS&E, KTH, Stockholm, SWEDEN.

We investigate a numerical model of Ostwald ripening in which matter is discretised. The model is based on transport by random walk and certain rules at the phase interfaces to mimic the continuous solution of the diffusion and moving boundary problem. In the limit of low volume fractions the results from our simulations agree quantitatively with the results predicted by the Lifshitz-Slyosov-Wagner theory. In contrast to the LSW model, the volume fraction of particles enters into our model as part of the diffusion problem and we may therefore shed light upon what happens when the volume fraction of particles increases.

Y8.22
COARSENING KINETICS OF COHERENT PRECIPITATES: DEPENDENCE ON VOLUME FRACTION. Venu Vaithyanathan, L.Q. Chen, Department of MS&E, Pennsylvania State University, University Park, PA.

Rate of coarsening of precipitates have been shown to depend on volume fraction for many alloy systems. The coarsening rate dependence on volume fraction for ordered γ' precipitates in Ni-Al alloys, with significant lattice misfit, is not very clear. Experimental results on Ni-Al alloys are contradictory. We try to extract the coarsening kinetics dependence on volume fraction of γ' 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. Gemperlová[1], A. Jacques[3], M. Janeãek[2], T. Vystavâl[1], A. Gemperle[1], N. Zárubová[1]. [1]Institute of Physics AS CR, Na Slovance, CZECH REPUBLIC. [2]Faculty of Mathematics and Physics, Charles University, Praha 2. [3]Laboratoire de Physique des Matériaux, Ecole des Mines, Cedex, FRANCE.

Previous studies of dislocation interactions with grain boundaries (GBs) on quasi-macroscopic scale by *in situ* SR X-ray topography on Fe-4at%Si symmetric nearly $\Sigma 3$ ([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 repulsive 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 $\Sigma 3$ misorientation and the GB plane $(\bar{1}1\bar{2})_I/(\bar{1}1\bar{2})_{II}$ had the deviation from the exact coincidence in one-degree range. The specimens had the form of platelets 1.7x5.5mm and thickness 0.1±0.02mm. The boundary passed through the hole in the centre. The specimen normals were $[3\bar{1}1]_I/[113]_{II}$ and $m[22102]_I/[544]_{II}$. The tensile axes were chosen to promote slip transmission of dislocations with both primary Burgers vectors $[1\bar{1}\bar{1}]_I/[1\bar{1}\bar{1}]_{II}$ and slip planes parallel in the two grains. The specimens were observed during straining under bright field diffraction conditions using different diffracting 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 20° 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 sub-grain boundary is formed in the other grain when the angle between the slip plane and GB is about 49°. The dense net 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 202/98/1281) and of PICS (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. Kazaryan, 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, Dept of MS&E, Columbus, OH.

The effect of pore drag on grain boundary mobility is investigated using a diffuse-interface phase field model. The model takes into account various diffusion mechanisms without imposing any a 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 spacing. Computer simulation results illustrating the effect of each of these parameters on grain boundary mobility as well as on the morphology of the interacting grain boundary and pores will discussed.

Y8.26
NUCLEATION OF PORTEVIN-Le CHATELIER BANDS IN PLASTICALLY DEFORMING ALLOYS. P. Sapalidis, Lab of Mechanics & Matls, Aristotle Univ of Thessaloniki, Thessaloniki, GREECE; M. Zaiser, Max-Planck Inst fur Metallforschung, Inst fur Physik, Stuttgart, GERMANY; P. Hahner, TU Braunschweig, Inst fur Metallphysik & Nukleare Festkorperphysik, Braunschweig, GERMANY; E.C. Aifantis, Lab of Mechanics & Matls, Aristotle Univ of Thessaloniki, Thessaloniki, GREECE.

The Portevin–Le Châtelier (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 'slaved' 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 DISLOCATION MOVEMENT IN 2D SYSTEMS: BRITTLE AND DUCTILE REGIMES. M. Robles, 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 crack, by 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. Eggleston and P.W. Voorhees, Dept. of MS&E, Northwestern Univ., Evanston, IL.

Interfacial energies in many materials are strongly anisotropic. In such cases the Wulff shape can 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 inefficient 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 *Y9.2
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, Oersted Laboratory, Niels 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 anisotropy depends on size. This behavior can be understood as a result of their oscillatory residual strain energy, and an edge energy term that is found to be mostly 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 ledges in order to reach the true equilibrium shape. Analysis of the size dependent shape evolution indicates a roughening transition at about 550C. The observations described in this work give direct evidence of the overriding effect of edges and ledges 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 Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy under Contract No. DE-ACO3-76SFOOO98.

9:30 AM Y9.3
PHASE DIAGRAM, INTERFACIAL FREE ENERGIES, AND TEMPERATURE DEPENDENCE OF COHERENT MICROSTRUCTURE IN Al-Sc ALLOYS. Vidvuds Ozoliņš, Dept. of Thin Film and Interface Science, Sandia National Laboratories, Livermore, CA; Mark Asta, Dept. of MS&E, Northwestern Univ., Evanston, IL.

Thermodynamic properties andcoherent microstructure of 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 almost a factor of thirty. Using atomistic Monte Carlo simulations we study shapes of coherent precipitates of the intermetallic $L1_2$ Al_3Sc phase in Al matrix as functions of precipitate size and temperature. We find a strong preference for forming cubic Al_3Sc 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
Chairs: Michael W. Finnis and Douglas L. Medlin
Thursday Morning, November 30, 2000
Independence E (Sheraton)

10:15 AM *Y10.1
STOICHOIMETRY AT THE OXIDE-METAL INTERFACE. Michael W. Finnis, Ali Alavi, Iskander G. Batyrev, Queen's University of Belfast, Atomistic 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 sulphur in the growth and adhesion of oxide scales. An equivalent formulation of the problem is to ask what is the interfacial free energy as a function of stoichiometry. We outline a method for doing such calculations at the atomic scale, illustrating it by discussing the relative free energies of variously terminated Nb/alpha-alumina(0001) interfaces which were obtained from first-principles, plane-wave pseudopotential calculations[1].// [1] I.G. Batyrev, A.Alavi 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 HETEROPHASE INTERFACES. Dieter Isheim and David N. Seidman, Northwestern University, Department of MS&E, Evanston, IL.

We are studying heterophase interfaces between molybdenum nitride precipitates and an α-Iron matrix on a nanoscale by electron and atom-probe field-ion microscopies. Internal nitridation is achieved by annealing specimens of an Fe-2at.%Mo-0.4at.%Sb alloy in an NH_3/H_2 atmosphere. Nitridation at temperatures between 550 and 650°C creates molybdenum nitride precipitates with a variety of morphologies and therefore a variety of heterophase interfaces. At lower temperatures, thin platelet-shaped precipitates a few atomic layers in thickness form, while nitridation at higher temperatures results preferentially in a coarser microstructure containing thicker platelets and spheroid-shaped precipitates. A higher level of Sb segregation is observed at the heterophase interfaces of the larger and thicker precipitates. The loss of coherency, that is the generation of misfit dislocations, is significant for the formation of these more massive precipitates. The relation between misfit dislocations at these heterophase 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 $\Sigma5$ (310)/[001] SYMMETRIC TILT GRAIN BOUNDARY IN COPPER DOPED ALUMINUM AND SILVER DOPED COPPER. Jürgen M. Plitzko, 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 segregation in a copper $\Sigma5(310)/[001]$ symmetric tilt grain boundary (STGB). The metals were doped with 1at% of copper in the aluminum and 1at% silver in the copper crystals. Bicrystals were produced by diffusion bonding and subsequent annealing to encourage segregation to the grain boundary. For comparison, we used bicrystals of the pure metals in the same misorientation. The atomic structure of the $\Sigma5$ (310)/[001] STGB for the different metal systems was modeled with atomistic potentials based on the Embedded Atom Method (EAM). The theoretical calculations of the interface structure indicate that the Cu and the Ag atoms segregate to distinct atomic sites at the interface. Investigations were performed using high-resolution electron microscopy (HRTEM) in combination with image simulation. We also used focal-series reconstruction to validate the predictions of the EAM model. Focal-series reconstruction can provide not only detailed information on the atomic structure but can also provide chemical information related to the projected potential (atomic number) of the elements under investigations. 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 findings regarding the two 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
CHARACTERIZATIONS OF LAMELLAR INTERFACES FOR A PST-TiAl ALLOY BY AN ANALYTICAL SCANNING TRANSMISSION ELECTRON MICROSCOPE. Wei Zhao and David E. Luzzi, University of Pennsylvania, Department of MS&E, Philadelphia, PA.

Polysynthetically-twinned (PST) TiAl with a gamma-alfa2 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 tertiary elements to the binary TiAl system appear to improve the ductility of the material from room- to mid-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 TiAl (Al-49.3 % at.) and related ternary TiAl X 0.6% at. (X = Ni, Cu, Mn, W, and Ta) alloys are characterized by high-resolution (JEOL 4000) and field emission analytical transmission electron microscopy (JEOL 2010F), coupled with energy dispersive x-ray spectroscopy, elmental mapping and line-scan techniques. TEM samples are prepared from the TiAl single crystals, which were grown by an ASGAL optical floating-zone directional solidification system. Twins, stacking faults, and defects at interfaces, as well as the segregation of tertiary elements to the lamellar boundaries, are characterized.

11:30 AM Y10.5
ATOMIC AND ELECTRONIC STRUCTURE OF HIGH PURITY SiC GRAIN BOUNDARY. Eriko Takuma, Hideki Ichinose, 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 atomic-resolution high voltage transmission electron microscope (ARHVTEM). Owing to excellent resolution of this ARHVTEM at the Scherzer defocus condition, we can directly distinguish atomic sites of Si and C in the grain boundary from the image contrast; Si atomic column appears in a darker spot and C atomic column appears in a thinner spot. Mainly observed boundary was parallel to (0001) plane of one crystal and to (1-102) plane of the other, rotated by 70.5 degrees around ¡11-20¿ axis. A structural unit of this boundary consisted of 5-7-6-6-6-6-membered rings. In the 6-membered rings unlike atoms faced to each other (Si faced to C). Only the atomic pair between the 5-membered ring and the 7-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 5-membered ring and the other was in the 7-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 electron energy loss spectroscopy (EELS) and the first-principles molecular dynamics method.

SESSION Y11: INTERFACE AND DISLOCATION INTERACTION

Chairs: Mark Aindow and Douglas L. Medlin
Thursday Afternoon, November 30, 2000
Independence E (Sheraton)

1:30 PM *Y11.1
INTERFACIAL LINE-DEFECT MECHANISMS IN SHAPE-MEMORY AND SUPER-ELASTIC ALLOYS. R.C. Pond, S. Celotto and P. Fox, MS&E, Department of Engineering, University of Liverpool, Brownlow Hill, Liverpool, UNITED KINGDOM.

Alloys which exhibit shape-memory (S-M) and super-elastic (S-E) 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-dominant and pure-shear deformation in the two types of interfaces respectively, and is diffusionless in both cases. Moveover, there is considerable experimental evidence that the passage of interfacial dislocations along these interfaces is the mechanism by which the deformation 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 S-M and S-E 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 was approached 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 transformation dislocations since it is necessary to demonstrate that 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 line-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 PM Y11.2
HREM STUDY OF INTERFACES IN A DUPLEX STAINLESS STEEL. Huisheng Jiao, Malcolm Hall, Univ of Birmingham, School of Metallurgy and Materials, Birmingham, UNITED KINGDOM; Robert Pond, Univ of Liverpool, Dept of MS&E, Liverpool, UNITED KINGDOM; Mark Aindow, Univ of Connecticut, Dept of Metallurgy and Materials Engineering, Institute of Materials Science, Boston, CT.

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 measurements of the orientation relationship (OR) between gamma (FCC) and alpha (BCC) showed it to be near Kurdjumov-Sachs (K-S) with a mis-orientation of 1.4 degrees between (101)alpha and (1-11)gamma, and 0.3 degrees between [11-1] alpha and [10-1] 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 335gamma and 011gamma. Both of these interfaces were semi-coherent 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 characterised by using circuit mapping procedures to analyse HREM images obtained with the interfaces edge-on, and comparing these data with what we would expect on the basis of the topological theory of interfacial defects. In this paper, an overview of these observations will be presented. It will be shown that by using these results together with a suitable reference 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 Y11.3
SLIDING BEHAVIOUR OF SYMMETRIC TILT BOUNDARIES WITH SPECIAL, NEAR-SPECIAL AND NON-SPECIAL MISORIENTATIONS IN ZINC BICRYSTALS. Askar Sheikh-Ali, Jerzy Szpunar, Dept of Metallurgical Engineering, McGill University, Montreal, QC, CANADA.

Observations of grain boundary sliding along symmetric tilt coincidence Sigma=91122 and three boundaries deviated at different angles from coincidence misorientation have been made in zinc bicrystals. The coincidence boundary and boundaries whose deviation does not exceed approx6 degrees slide and migrate in a coupled manner predicted by the DSC-dislocation model. The boundary whose deviation exceeded approx6 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 a boundary to slide and migrate in a fixed ratio is an important criterion for its specialness.

2:30 PM Y11.4
THE EFFECT OF EXTENDED SUPERDISLOCATION / DOMAIN BOUNDARY INTERACTIONS IN ORDERED INTERMETALLIC COMPOUNDS. T.S. Rong, I.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 [1-3]. 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 area created once the whole superdislocation has passed through. In this paper we will present an overview of this model. It will be shown that if 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 more significantly with domain size than is predicted by previous models. It will also be shown that these effects would 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 existing models. Further implications of the model in terms of the generation of planar slip and uncoupled superpartial dislocations will be discussed. 1. Cottrell, A.H., 1954, Relation of Properties to Microstructure, ASM Monograph, 131. 2. Ardley, G.W., 1955, Acta metall., 3, 525. 3. Marcinkowski, M.J., and Fisher, R.M., 1963, J. Appl. Phys., 34, 2135.

3:30 PM *Y11.5
"DISLOCATION-GRAIN BOUNDARY" INTERACTION IN NICKEL BICRYSTALS AND EVOLUTION OF THE RESULTING DEFECTS UNDER THERMAL TREATMENT. Louisette Priester, Sophie Poulat, Université Paris XI, LEMHE, Orsay, FRANCE; Brigitte Décamps, CNRS, LCMTR, Thiais, FRANCE; Jany Thibault, CEA, DRFMC, Grenoble, FRANCE.

The interactions between lattice dislocations and grain boundaries (GBs) have been studied in nickel bicrystals grown by solidification along the $< 110 >$ axis. Three types of GBs, according to their energy, have been investigated : singular $\Sigma 3$ {111}, vicinal near $\Sigma 11$ {311} and general near $\Sigma 11$ {332} 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 $\Sigma 3$ {111} GB. It consists in a dissociation within the GB of the trapped lattice dislocation followed by the emission of one partial in the neighbouring crystal. But, most often, the absorbed lattice dislocations or extrinsic grain boundary dislocations (EGBDs) react 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 PM *Y11.6
DISLOCATION DYNAMICS IN INTERMETALLIC, OXIDE DISPERSION STRENTHENED (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 $MoSi_2$, 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 jerkiness of their motion. Both are specific of the different mechanisms controlling the dislocation mobility. Straight dislocations moving viscously 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 at the action of localized obstacles, where the bowing 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 diffusing species can be quite different, alloying components or intrinsic point defects like vacancies and antisite defects existing in the lattice or only in the dislocation cores. It may also be conservative climb between partial dislocations separated by a climb dissociation. 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 PM 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-base 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 PM Y11.8
DISSOCIATION OF AND 9R PHASE FORMATION IN A HIGH ANGLE GRAIN BOUNDARY VIA SEPARATION OF INTERFACIAL DISLOCATIONS. Stephen M. Foiles, Sandia National Laboratories, Albuquerque, NM; Doug L. Medlin, Sandia National Laboratories, Livermore, CA.

Au films 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 9R phase at the boundary. This is similar to the 9R phase formation observed previously for $\Sigma 3$ boundaries. However, in this case the dissociation is observed to occur at a high angle boundary which has approximately a $\Sigma 99$ 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 $\Sigma 3$ case.