TECHNICAL PROGRAM

Third International Conference on Grain Growth (ICGG-3)

MONDAY AM

Plenary Session

Monday AM — Room: McConomy Auditorium (1st floor)
June 15, 1998 — Location: University Center

8:45 AM WELCOME

9:00 AM PLENARY LECTURER
MODELS OF GRAIN GROWTH: W. W. MULLINS[1]; [1]Carnegie Mellon University, Materials Science and Engineering, Pittsburgh, PA USA

A brief history of the principal models of grain growth induced by grain boundary energy reduction will be presented. These include stochastic models and deterministic models, both vertex and curvature based. The theoretical foundations of these models will be examined and compared, with emphasis on curvature models. A general theorem based on curvature driven growth will be presented that permits the deduction of relative grain boundary mobilities from a given experimental microstructure. Some new theoretical results for the two dimensional uniform grain boundary model, based on the concept of statistical self-similarity, will be presented and used to analyze the Hillert theory in relation to simulation data. Finally, some discussion of exaggerated grain growth that results from non-uniform boundaries will be given.

10:00 AM BREAK

Vertices

Monday AM — Room: Rangos Hall-Room 1 (2nd floor)
June 15, 1998 — Location: University Center

10:30 AM
THE EFFECT OF INITIAL GRAIN SIZE DISTRIBUTION ON ABNORMAL GRAIN GROWTH: A MODEL BASED ON HILLERT'S FORMULATIONS: WILLIAM E. BENSON[1]; John A. Wert[1]; [1]University of Virginia, Department of Materials Science and Engineering, Thornton Hall, MSE Building, Charlottesville, VA 22903 USA

A model that describes the temporal evolution of a grain size distribution (GSD) has been used to analyze the effect of initial GSD on grain growth. The model is based on the work of Hillert and Hunderi and Ryum. Initial GSDs were synthesized by superposing two steady state GSDs with different critical radii. Two parameters describe the initial deviation from steady state: umax is the ratio of the largest grain radius to the critical grain radius and F is the fraction of grains larger than twice the critical radius. The evolution of initial GSDs that deviate from steady state is then modeled. In the absence of a pinning force from particles, a transient period of abnormal grain growth occurs as the GSD evolves toward steady state for all initially non-steady state GSDs with umax > 2. In the presence of particles, grain growth stagnation occurs. When the pinning force associated with particles is removed after stagnation, a transient period of abnormal grain growth occurs during the initial stage of evolution to a steady state GSD. In both cases, an index is proposed that predicts the extent of excess grain growth from characteristics of the initial GSD.

10:50 AM
EFFECT OF SOLID-STATE WETTING ALONG GRAIN BOUNDARY OR TRIPLE JUNCTION ON ABNORMAL GRAIN GROWTH: NONG M. HWANG[1]; Sung B. Lee[1]; Chan H. Han[1]; Duk Y. Yoon[1]; [1]Korea Res Inst. of Standards & Science, Microstructure Science Group, P.O. Box 102, Ysung-gu, Daedok Science Town, Taejon 306-600 Korea

When the grain boundary energy is anisotropic, a grain can penetrate along the grain boundary or the triple junction by solid-state wetting. Grain boundary wetting will take place at the triple junction when the sum of the two grain boundary energies is smaller than the other grain boundary energy. The triple junction wetting can also take place in a 3-dimensional grain structure starting at the four grain corner. It was shown by 3-dimensional Monte Carlo simulation that abnormal grain growth can be induced by such solid-state wetting under a realistic condition in anisotropic grain boundary energy. The experimental evidence, which shows the possibility of abnormal grain growth by such solid-state wetting, was pursued in an initial stage of abnormal grain growth in an Fe-3%Si alloy. Among the matrix grains near abnormally growing grains, three-sided and four-sided grains have the grain boundaries with curvatures convex toward a center of the grains, indicating that they are not shrinking but growing against the large grains surrounding them. The extremely high frequency of island grains was observed in the initial stage of abnormal grain growth. These microstructural features imply abnormal grain growth by solid-state wetting.

11:10 AM
ON DRIVING AND RETARDING FORCES OF RECRYSTALLIZATION IN METAL MATERIALS: V. V. GUBERNATOROV[1]; [1]Ural Branch of RAS, Institute of Metal Physics, Yekaterinburg Russia

Certain issues associated with driving and retarding forces of recrystallization have been considered. It is shown that in most cases the main driving force of the primary recrystallization is the boundary energy. A mechanism is proposed for the formation of segregations and particles of surplus (secondary) phases at the boundaries during recrystallization. This mechanism consists in the following. The moving boundaries carry a large amount of impurities when the grains collide one another, two moving boundaries form one stationary boundary, which accumulates the impurities carried by both moving boundaries. If the number of impurities exceeds the dissolution limit at this boundary, the surplus impurities will precipitate as particles of excess phases.

11:30 AM
INFLUENCE OF PINNING FORCE ON ABNORMAL GRAIN GROWTH EVOLUTION: V. YU NOVIKOV[1]; [1]Moscow Institute of Steel and Alloys, Treptower Str. 74 d, Hamburg D-22147 Germany

Pinning force is one of the factors leading to the inhibition of normal grain growth and to development of abnormal grain growth (AG). The influence of its magnitude and behavior on AG has not been systematically explored. The present study is one of the first attempts to investigate the influence of pinning force on AG evolution in polycrystals having different initial rnicrostructures. The work was carried out by means of computer simulation. The effects of the initial magnitude of pinning force and its reduction rate were investigated. Experiments at a constant pinning force showed that the pinning force magnitude necessary for AG triggering is greatly affected by the initial microstructure. At a decreasing pinning force, AG evolution depends on both the initial microstructure and the initial magnitude of pinning force. In a coarse-grained polycrystal, AG develops completely at a certain value of the pinning force reduction rate. It is interrupted at a

smaller rate, and it appears suppressed at a higher rate. Such a behavior is qualitatively the same in the studied range of the initial pinning forces. In a fine-grained polycrystal, AG development at a relatively low rate is identical to that described above. However, at an increased value of the initial pinning force, AG in such a polycrystal evolves completely in a wide range of reduction rates of pinning force. Data on the effect of an increased grain-size non-homogeneity on AG development are also given.

11:50 AM LUNCH

Topology

Monday AM
June 15, 1998

Room: Rangos Hall-Room 3 (2nd floor)
Location: University Center

10:30 AM

TOPOLOGICAL PROCESSES AND THE KINEMATICS OF GRAIN GROWTH IN THREE DIMENSIONS: R. T. DEHOFF[1]; [1]University of Florida, Dept. of MS&E, P.O. Box 116400, Gainesville, FL 32611 USA

From a geometrical point of view grain growth is the coarsening of a space filling tessellation. The total surface area of the tessellation and the number of cells it encloses decreases as the average cell volume increases. Elements of the facets in the cell structure move toward their centers of curvature dragging their bounding triple lines and quadruples point along. At intervals local configurations in the surfaces, lines and nodes in the network achieve a critical geometric condition and a local topological change occurs in the network. These topological processes fall into three classes: Class I: Disappearance of small, simple (tetrahedral) cells; Class II: Connection between two previously disconnected grains; Class III: Disconnection of two previously connected grains. This presentation explores the connection between changes in the metric properties of the tessellation and these topological processes. It is demonstrated that the decrease in grain surface area which is grain growth is derived almost completely from the losses in area directly associated with these topological processes.

10:50 AM

GRAIN BOUNDARY STATISTICS AND TOPOLOGICAL CHARACTERISTICS OF THE GRAIN BOUNDARY NETWORKS: V. Y. GERTSMAN[1]; J. A. Szpunar[1]; [1]McGill University, Dept. of Metallurgical Engineering, 3610 University Street, Montreal, PQ, H3A 2B2, Canada

Statistical characteristics of the grain boundary ensembles in statically recrystallized materials susceptible to annealing twinning have been studied. These include: the frequencies of occurrence and relative lengths of different grain boundary types, and the frequencies of triple and multiple junctions. The influence of grain growth on the statistical parameters of the interface network and relationships among these characteristics are analyzed. It is shown that while some microstructural characteristics could be considered as almost independent of each other, relationships between some other parameters depend on the topology of the grain boundary network. An example of the former type of relations is that the relative lengths of different types of grain boundaries could be different in the microstructures with similar fractions of grain boundary types, i.e. similar grain boundary character distributions. At the same time, the grain boundary character distribution is dependent on the connectivity of the grain boundary network, for example, on the presence of isolated embedded grains and multiple junctions in addition to triple junctions. In the case of an idealized grain boundary network consisting entirely of triple junctions, there are rigid relationships between the statistical characteristics of the grain boundary network. Experimental data accumulated to date have been analyzed and it has been shown that for the class of materials under consideration such an idealized situation is hardly applicable in many experimental cases.

11:10 AM

SELF-SIMILARITY AND LOGNORMAL SIZE DISTRIBUTIONS IN COARSENING SYSTEMS: THE CASE OF NANOCRYSTALLINE ZIRCONIA: Tomas Chraska[1]; ALEXANDER H. KING[1]; Christopher C. Berndt[1]; [1]State University of New York at Stony Brook, Department of Materials Science & Engineering, Stony Brook, NY 11794-2275 USA

A persistent question about grain growth and other particle coarsening phenomena concerns the origin of the lognormal particle-size distribution which is almost universally observed. Does this distribution occur simply because it is the starting distribution for a self-similar form of growth, or is it intrinsically preferred for other reasons? We present some observations made during the coarsening of nanocrystalline zirconia particles, which are germane to this question. Zirconia undergoes a phase transformation when the particle size is of the order of 15 nm, for reasons associated with the surface energy, and the occurrence of this phase transformation produces a sudden change in the driving force for coarsening. Grain size distributions below the critical size for the transformation are lognormal, but as the transformation occurs, the size distribution changes to a markedly less skewed form. The development of this distribution is followed to establish whether it grows self-similarly, or returns to log-normality once normal driving forces are restored after the phase transformation is complete.

11:30 AM

STATISTICAL CHARACTERIZATION OF GRAIN BOUNDARY NETWORKS IN METAL INTERCONNECTS: X. J. XUE[1]; S. K. Kurtz[1]; K. J. Kozaczek[2]; D. S. Kurtz[2]; [1]The Pennsylvania State University, University Park, PA 16802 USA; [2]Advanced Technology Materials, Inc., State College, PA 16801

In the integrated circuits (IC's), aluminum alloy fine lines are widely used to provide electrical connections. These fine lines are patterned from a blanket thin film deposited on a dielectric material layer, which is on the top of a silicon wafer. In state-of-the-art semiconductor technology, these interconnects have width and thickness of less than 1 μm and are encapsulated by multiple layers of dielectric materials, such as TiN. Since the median grain size is larger than the width of the interconnects, a bamboo-like micro structure is observed. This structure is made up largely of a sequences of individual grains interspersed with some multiple-grain regions (i.e. polygranular sections), grain boundary triple points etc. With the increase of component density and decrease of interconnect size in IC's the reliability issue becomes increasingly important. As a large portion of failure in IC's are due to malfunction of electrical interconnections, the failure mechanisms of interconnects during fabrication and service have been investigated for more than thirty years. Electromigration, stress-induced voiding and hillock formation, and corrosion are known as the main causes for such failures. Recently, accumulated evidence shows that interconnect failures are strongly related to the statistical features of the grain boundary network and crystallographic orientation of the individual grains [Kang96J]. An accurate microstructural model for the interconnects is thus fundamental for successfully predicting the lifetime of interconnects. In this paper, we discuss the statistical characterization of this grain boundary network in the fine line interconnects by supposing that each grain has a columnar structure in the direction normal to the wafer. By analyzing a number of stripes cut from a 2-D Laguerre tessellation, the dependence of the interconnect grain size distribution on the line width and the grain size distribution parameters of the original blanket thin film is determined. The distribution of grain boundary triple junctions, the distribution of polygranular section lengths, and the correlation of grain topology classes are studied based upon the same sampling. These computer simulation results are compared with experimental results [Sanchez97], and suggest that a narrow stripe cut from a 2-D Laguerre tessellation can serve as a useful mesoscopic model which correctly reflects the statistical topology of actual grain boundary network in fine line interconnects.

11:50 AM LUNCH

MONDAY PM

Pinning-1

Monday PM Room: Rangos Hall-Room 1 (2nd floor)
June 15, 1998 Location: University Center

1:30 PM INVITED PAPER

GRAIN GROWTH IN TEXTURED MATERIALS: H. J. BUNGE[1]; [1]Institut fur Metallkunde un Metallphysik, Technische Universitat Clausthal, Clausthal, Zellerfield D-38678 Germany

Grain growth is driven by the energy of grain boundaries, the movement of which depends also on mobility. These two fundamental quantities depend on five grain boundary parameters, i.e. misorientation of neighbouring grains and crystallographic orientation of the boundary normal direction. Hence, grain growth depends essentially on the crystallographic orientations of all grains, i.e. the texture and the orientation pair correlation, i.e. the MODF, besides many geometrical structure parameters such as grain size and number of neighbors. Grain growth is virtually always accompanied by texture changes. The earliest results concerned sharpening of the cube texture. Later on also shift of the cube texture as well as the occurrence of completely new texture components was observed depending (among others) on the spread width of the preferred orientation. Experimental investigations in many materials with many different types of textures confirm this general result. A second general (although less well established) result is larger average grain size of the growing texture components compared with the vanishing ones. Modelling of the grain growth process must take the stochastic nature of all parameters of the polycrystalline structure into account. This has been done in two different ways; i.e. statistical averages are taken either *before* or *after* carrying out the growth model. (In a somewhat misleading terminology only the first type of models have been called "statistical" models.) Particularly we shall consider here a statistical model based on the average grain boundary area and average length of grain edges of a model grain of size r and orientation g. Boundary area and length of edges define the resultant driving force which may either be positive or negative. Both, inwards and outwards pulling boundaries, may have different average energies as well as mobilities depending on the orientation g of the grain, the orientation distribution function ODF, as well as the orientation pair distribution MODF. Crystal orientation g must be considered in steps small enough to represent the (steep) variabilities of boundary energy and mobility. This means particularly that we must distinguish orientations within texture "components" which often have half-widths (FWHM) in the order of 20 degrees. Grain growth can be observed experimentally in a range of ~1:10 with respect to grain size, this means l:1000 for the volume fractions. Hence, strictly speaking the texture (ODF) must be considered with an accuracy of 0.1% which is, with the present experimental technique, not yet possible. together. Hence, the basic quantity is (at least) the four-dimensional orientation-size distribution (rather than the three-dimensional ODF and the one-dimensional grain size distribution). This requires new experimental investigations on this basis using the new orientation scanning technique.

2:10 PM

GRAIN GROWTH SIMULATION IN 2 DIMENSIONS IN THE PRESENCE OF PARTICLES: D. WEYGAND[1]; Y. Brechet[1]; J. Lepinoux[1]; [1]McMaster University, 1280 Main St. West, Ontario 00229 Canada

A 2 dimensional Vertex model based on Kawasaki's approach is developed in order to study' the influence of particles on the grain growth behaviour. We discretized the GB's by introducing supplementary (virtual) vertices. This allows to respect the equilibrium condition at the triple points and to model the pinning and depinning process of the particles. The individual depinning force in the 2 dimensional model is varied in order to simulate the influence of the size of the particles. The relation between the particle density, the force for depinning and the final mean grain size and grain size distribution is explored. The observed grain growth behaviour can he divided in different classes (import ant pinning force low pinning force and intermediate pinning force). For high depinning forces the mean radius $< r >_{max} \chi$ of the pinned structure follows roughly $< r >_{max} \chi$ 1/ N where N is the particle density and an important fraction of the pinned particles are located at the triple points or close to them. For low pinning forces the observed behaviour suggest that the saturation radius behaves as $< r >_{max} \chi N_{\alpha}$ with α — -1, (Zener limit). The simulated grain growth dynamics in presence of particles can be described by a simple "mean field" law $dr/dt \chi (1/R (1/R_{Rmax})$.

2:30 PM

MICRO-PATTERNING AS A TOOL FOR INVESTIGATING COARSENING PHENOMENA IN THIN FILMS: JEFFERY W. BULLARD[1]; Mohan Menon[1]; [1]University of Illinois at Urbana-Champaign, Department of Materials Science & Engineering, 1304 West Green Street, Urbana, IL 61801 USA

The dynamics of capillary-driven and stress-driven coarsening among thin film islands are influenced by several microstructural variables, including interphase boundary energies and lattice mismatch. The kinetics of local interface motion in such systems also depends on the diffusion field, which in turn is likely to be determined by volumes and spacings of nearby domains. Geometric correlations and rate-controlling material transport mechanisms during domain coarsening could be investigated in detail if experimental techniques existed for isolating microstructural variables such as the initial volume distribution and spacings of domains. We will discuss the use of micro contact printing for patterning thin film islands, and will demonstrate its use as a new way to examine the evolution of model heterophase thin film systems. Results will be presented for production and annealing of MgO thin film islands on spinel single crystals. The evolution of the system will be discussed in terms of both length scales and of spatial correlations among growing and diminishing islands, and the results will be used to infer the rate-controlling mass transport mechanism for coarsening of MgO on spinel.

2:50 PM INTERACTIVE SESSION: EXHIBITS

3:50 PM

SECOND PHASE INHIBITED GRAIN GROWTH: B. R. PATTERSON[1]; Y. Li[1]; [1]University of Alabama, Department of Materials and Mechanical Engineering, Birmingham, AL 35213 USA

Microstructural relationships observed during second phase inhibited grain growth will be reviewed. In particular the influence of the volume fraction, mean intercept and surface area of second phase and the degree of contact, R, between grain boundary and second phase will be addressed. The influence of grain growth temperature, material type, solid vs. porous second phase, and second phase mobility on R and the path of microstructural change will be addressed. It will be shown that commonly observed variations in the volume fraction exponent are the result of variations in R with volume fraction, f. An exponent value of unity results when the term R*f is used in Zener-type equations to describe the effective volume fraction of second phase at the grain boundary.

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COMPUTER MODEL FOR SIMULATING THE DIFFUSION PROCESS IN SOLIDS: H. LI[1]; J. A. Szpunar[1]; [1]McGill, Metallurgical Eng., 3610 University Street, Montreal, PQ H3A 2B2 Canada

Understanding of diffusion processes is of great importance for understanding of processes like oxidation, precipitation, creep, annealing and other processes. In this paper, a two dimensional computer simulation model is proposed to simulate the diffusion process in polycrystalline solids which contains defects such as point defects, dislocations and grain boundaries. In this model, the microstructure is described by unit cell with specified orientations and the grain size and grain shape are introduced to the model using available experimental data. One million of unit cells is used in the model. Each unit cell has a property defined by diffusion coefficient which represents the lattice

diffusion coefficient, or the dislocation diffusion coefficient or the grain boundary diffusion coefficient. Grain boundary diffusion coefficient is a function of grain boundary misorientation. The diffuison process is simulated with the Random Walk method. The output of simulation is presented as a normalized profile of oxygen concentration and a two dimensional contour map which display the distribution of diffusing species. Using this simulation model, the effects of grain shape, grain size and a role of various structure defects on the diffusion process can be studied. The model was tested using various experimental data and results obtained are compared with Fick's and Whipple's theoretical analysis.

4:30 PM
PARTICLE LIMITED GRAIN GROWTH: EXPERIMENTS AND SIMULATIONS: ROGER D. DOHERTY[1]; Kang Li[1]; M. P. Anderson[1]; [1]Drexel University, Department of Materials Engineering, Philadelphia, PA 19104 USA

The standard Zener particle drag model appears successful in describing the inhibition of pressurized grain boundary migration, for example in recrystallization. However, both experiments and simulations of the particle limited grain size in normal grain growth in three dimensions indicate a much smaller size, R 89 r / f 1/3, than the standard particle drag model's prediction of R 89 r/f. R and r are mean grain and particle radii and f is the volume fraction of particles. In addition, experiments show a very large scatter in the limiting grain size, for any given f and r. This scatter indicates that the grain size is controlled by additional parameters as well as f and r. Analysis of the simulations indicates, in grain growth in three as in two dimensions, that particles act, not as a frictional drag to boundary motion, but more fundamentally to remove the boundary curvature that drives grain growth. In confirmation of this idea simulations indicate, as predicted by the curvature removal model, that the final grain size is strongly determined by the initial grain size. In addition, since inhibition of abnormal grain growth appears to be correctly described by the Zener analysis, the present model successfully predicts the occurrence of abnormal grain growth in microstructures with both a small initial grain size and a very low volume fraction of particles.

4:50 PM ADJOURN

MONDAY EVENING
GATEWAY CLIPPER CRUISE

Grain Growth Theory

Monday PM
June 15, 1998

Room: Rangos Hall-Room 3 (2nd floor)
Location: University Center

1:30 PM INVITED PAPER
TOPOLOGICAL RELATIONSHIPS IN MICROSTRUCTURES AND THEIR APPLICATION TO A RIGOROUS STATISTICAL THEORY OF GRAIN GROWTH: K. LÜCKE[1]; R. Brandt[1]; G. Abbruzzese[2]; [1]RWTH Aachen, Institut fur Metallkunde & Metallphysik, Kopernikusstr 14, Aachen D-52074 Germany; [2]Centro Sviluppo Materiali, Terni Italy

Although C. S. Smith and J. V. Neumann had mentioned already that for a theoretical description of grain growth beside rate equations also topological relationships are required, no treatments of this subject can be found in literature. Only by the present authors some aspects of it have recently been derived. In the present work a survey over this new field being here called Topological Metallography is given. It mainly concerns (i) the description of space filling along a grain boundary (grain boundary symmetry), in particular volume conservation during boundary motion, (ii) correlation with respect to the frequency of neighboring grains of various sizes, (iii) correlation with respect to the frequency of neighboring grains of different orientations and (iv) relationships between size and the number of sides of a grain. Furthermore, for the case of random neighborhood correlations analytical expressions for the rate of grain growth could be derived.

2:10 PM
STATISTICAL THEORY OF GRAIN GROWTH IN THE PRESENCE OF ZENER AND ATOMS DRAG: G. ABBRUZZESE[1]; K. Lucke[2]; R. Brandt[2]; [1]CSM Terni Unit, v.le B. Brin, 218, Terni I-05100 Italy; [2]IMM -RWTH, Aachen Germany

Most of the grain growth processes in technical polycrystalline materials occur in the presence of restraining forces opposing the grain boundary movement generated by second phase particles and or by a certain amount of solute elements segregating the grain boundaries The mechanisms by which the restraining forces operate are quite well established however, their effects on grain growth kinetics are often discussed on heuristic basis and mostly considering a strongly simplified microstructure which typically do not allow to consider the various microstructural features playing a role on the kinetics of grain growth or on the conditions of abnormal growth effects. Here the approach of the statistical theory of grain growth is used and the effect of the grain growth inhibition is introduced at the very basic level of the single gram boundary. The calculation of the growth kinetics of a given grain is by summing up the various contributions of the surrounding grains in the presence of Zener or Atoms drag shows that the concept of only one critical radius, existing for the whole size distributions as it was introduced by Hillert is no longer valid. Instead for each grain size class I a well defined critical radius appears. The latter result has significant consequences, particularly in respect to the approaching; grain growth stagnation and the onset of abnormal grain growth. Simulations by this model show the details.

2:30 PM
COARSENING KINETICS OF INITIALLY FRACTAL GRAIN BOUNDARIES: P STREITENBERGER[1]; [1]Otto-von-Guericke-Universitaet Magdeburg, Inst fur Experimentl Physik, Postfach 4120, Magdeburg D-39016 Germany

A novel coarsening regime for serrated or rugged grain boundaries in single-phase polycrystalline materials is presented. The coarsening is characterized by a smoothing of the initially rough grain boundaries, where the time law of the smoothing kinetics, measured e.g. by the evolution of the profile roughness ρ of the grain boundaries, is given by the power law $\rho \cup t^{1-D2)12}.D_s$ (with $1 \leq D_s 2$) is the initially fractal dimension of the grain boundaries as it can be determined by the application of the concepts of fractal geometry to micrographs of plain sections of the grain ensemble. The time law is derived by an analytic model of self similar boundary coarsening based on the phenomenological assumption of a curvature driven relaxation of simplifying fractal-like grains. By application of optical and scanning electron microscopy over a wide range of magnifications, the model is tested experimentally by the measurement of the coarsening kinetics of initially fractal-like grain boundaries in pure Zinc and Titanium during isochronous as well as isothermal annealing. Additionally, a Monte Carlo simulation of the thermal relaxation of two-dimensional initially fractal grains is performed. The results of the simulation confirm the assumptions of the phenomenological model and are in good agreement with the annealing experiments.

2:50 PM INTERACTIVE SESSION: EXHIBITS

3:50 PM
A STATISTICAL THEORY OF GRAIN GROWTH FOR NON UNIFORM GRAIN BOUNDARIES: R. BRANDT[1]; G. Abbruzzese[2]; K. Lücke[1]; [1]RWTH, Aachen Germany; [2]Centro Sviluppo Materiali, Terni Italy

The basic statistical theory of curvature driven grain growth for 2D formulated by Abbruzzese and Lücke for uniform grain boundaries (GBs) is extended to the case of nonuniform GBs. A fundamental approach based on first principles is applied which considers also the mechanical

equilibrium conditions at the vertices determined by the pregiven specific energies of the three meeting GBs. The effect of texture on grain growth caused by the GB energies and mobilities depending on the orientation differences of adjacent grains is discussed by means of this theory. In contrast to the case of uniform GBs here not a single, but a set of several continuity equations and a set of growth rates, one for each texture component, is obtained. For the case of only 2 texture components the increase of grain sizes and the evolution of the texture has been predicted by simulations. The results show good agreement to experimental results in Al3%Mg alloys.

4:10 PM
REMARKS ON THE SIMULATION OF GRAIN BOUNDARY MOTION: D. L. KINDERLEHRER[1]; S. Ta'asn[1]; C. Liu[1]; F. Manolache[1]; [1]Carnegie Mellon University, Department of Mathematical Sciences, Pittsburgh, PA 15213 USA

The Mesoscale Interface Mapping Project requires the interrogation of vast numbers of triple junctions to infer the energy and mobility of the grain boundaries as functions of lattice mismatch and geometry. The relationships among these quantities are the force balances at the triple junctions, known as the Herring Relations or Young's Equation. In equilibrium these conditions hold as a result of stationary energy for the grain boundary network. However when the system is not in equilibrium, a situation present when seeking mobilities, these equilibrium conditions must be assumed. This is an assumption of the project. Is this justified? We show that assuming the Herring Relation at triple junctions leads to stable evolution to a stationary configuration. We then present simulations illustrating this and suggest some applications of them for the enhancement of the experimental program.

4:30 PM
COMPARISON OF ABNORMAL AND NORMAL GRAIN GROWTH: D. B. TITROV[1]; [1]Ural Branch of Russian Academy of Sciences, Physical-Technical Institute, Izhevsk, Russia 42600 USA

The velocity of the movement of the boundaries of the grains growing abnormally in the alloy Fe + 3%Si (secondary grains) is constant. The law of normal grain growth is parabolic. The velocity of abnormal grain growth is by 3 - 4 orders more than the initial velocity of normal grain growth. Besides that the orientations of the basic texture components change because of abnormal grain growth, but at normal grain growth do not change. The grain boundaries, triple junctions (TJ) and quadripartite joints (QJ) move during grain growth in polycrystals. Triple junctions are the specific linear polycrystal defects (as compared with dislocations in single crystals) where three grain boundaries are joined. Quadripartite joints are the specific polycrystal dot defects (as compared with vacancies in single crystals) where four triple junctions are joined. The role of vacancies at grain growth has been discussed. At normal grain growth the casual meetings of vacancies with quadripartite joints initiate relay races of displacement of atoms to the neighbour grains first through triple junctions, and then through grain boundaries. This is the reason of parabolic kinetics, small growth rate and stability of texture at normal grain growth.

4:50 PM ADJOURN

MONDAY EVENING
GATEWAY CLIPPER CRUISE

TUESDAY AM

Pinning-2

Tuesday AM
June 16, 1998

Room: Rangos Hall-Room 1 (2nd floor)
Location: University Center

8:30 AM INVITED PAPER
APPLICATIONS OF GRAIN GROWTH MODELING: ELISABETH HOLM[1]; C. C. Battaile[1]; M. D. Rintoul[1]; M. A. Miodownik[1]; [1]Sandia National Laboratory (TSNL), Physical & Joining Metallurgy, Mail Stop 1411, P.O. Box 5800, Albuquerque, NM 87185-1411 USA

Microstructure has generally been linked to materials performance via average microstructural parameters; for example, the Hall-Petch equation relates yield strength to average grain size. However, computer simulations of microstructural evolution generate grain structures which enable new capabilities in coupling microstructure to properties. At one level, simulations can provide realistic structures for examining the effects of complex polycrystalline geometry and topology on properties. For example, the minimum energy intergranular fracture surface of a polycrystal depends on the details of its grain structure. Polycrystalline mass transport, flaw initiation during plastic flow, and solid-state nucleation are also governed by the geometry, topology and connectivity 0 f grains. Another scientific and computational challenge involves linking materials response calculations to subsequent microstructural evolution. For example, coupling a microstructural evolution simulation to a polycrystalline finite element model elucidates the interdependence of grain growth and plastic flow in a polycrystal. Likewise, coupled simulations illustrate the connection between grain growth and microcracking during hot pressing of brittle ceramics.

9:10 AM
PHYSICAL AND COMPUTER SIMULATIONS OF GRAIN GROWTH IN A PINNED MICROSTRUCTURE: C. H. WORNER[1]; B. K. Kad[1]; P. M. Hazzledine[1]; [1]UES, Inc., Dayton-Xenia Road, Dayton, OH 45432 USA

Three methods are available for modeling two-dimensional grain growth and stagnation in the presence of Zener pins: analytical models, computer simulations and soap film simulations. The Friedel-Zener analytical model gives the same pinned structure as computer Potts simulations but gives no information on the kinetics of growth. Soap film simulations also give the same pinned structure and they display growth kinetics which agree closely with those in the Potts simulations. The upshot of the three models is that growth is a three-stage process with an incubation, or slow growth stage, followed by a steady state growth stage and finally gradual stagnation. In the steady state growth stage the grain diameter D is proportional to a power of the time t^p where p is close to 1/2. Once stagnation has occurred, the pinned grain size is proportional to a power of the volume fraction of pins f^q where q is also close to 1/2. In this paper the three models are compared for the case in which the pins are circular. The problems posed by the small deviations of p and q from their expected values of 1/2 are addressed. In addition, progress is reported, using all three modeling methods, towards extending the theory of Zener pinning to microstructures in which the pins have elongated shapes.

9:30 AM
A MONTE CARLO MODEL OF ZENER PINNING WHICH SHOWS AN f^{-1} DEPENDENCE: MARK ANDREW MIODOWNIK[1]; [1]Sandia National Labs, Albuquerque, NM 87185-0340 USA

A novel 3D Monte Carlo model of Zener Pinning has been developed. It differs from previous MC models in that it does not simulate polycrystalline grain growth. Instead the movement of a single boundary through an array of particles is simulated. By incrementally increasing the volume fraction of particles, the boundary is eventually

pinned. This defines the Zener criterion and enables the volume fraction dependence of the model to be determined. The value of this approach is that no limit is imposed on either the volume fraction, f, of particles or their size. Simulations have been carried out over a range of volume fractions from f=0.01 to f=0.2. for particles with volumes up to 27 sites. The pinning force exerted by particles on a boundary is related to the characteristic shape during bypass, the so called 'dimple'. When the simulation temperature T=0, dimples are not formed, the boundaries experience an artificially strong pinning force and the model exhibits an $f^{-1/2}$ dependence. When T is greater than a critical value, dimples are formed and the model shows an f^{-1} volume fraction dependence. The implications of this result for previous MC models of Zener pinning is discussed.

9:50 AM INTERACTIVE SESSION

11:00 AM INVITED PAPER

SOME THEORETICAL CONSIDERATIONS ON THE ABNORMAL GRAIN GROWTH DEVELOPMENT FROM UNIFORM GRAIN SIZE DISTRIBUTIONS: P. R. RIOS[1]; [1]Universidade Federal Fluminese, Escola de Engenharia Industrial Metalúrgica de Volta Redonda Av. dos Trabalhadores, 420 Vila Santa Cecília, Volta Redonda , RJ 27260-740 Brazil

Most of the existent models on abnormal grain growth assume that a large preexistent grain is already present. However abnormal grain growth is often found to develop from uniform grain size distributions in which no obvious initial heterogeneity is present. In this paper some possible causes for an abnormal grain to develop from uniform grain size distributions are examined. First a local fluctuation in the pinning force is shown to be able to cause abnormal grain growth both in the presence of stable and unstable particles. Second it is shown that a higher grain boundary mobility could also cause abnormal grain growth to develop from uniform grain boundary distributions. The circumstances in which it is not necessary for a high mobility to be maintained for abnormal grain growth to continue are also discussed. Based on the theoretical analysis it is concluded that the local environment, such as a locally lower pinning force or a higher mobility due to favorable orientation, is a key factor in the development of abnormal grain growth from uniform grain boundary distributions.

11:40 AM

INFLUENCE OF ORIENTATION PINNING ON THE GOSS-TEXTURE IN Fe-3%Si ELECTRICAL STEEL: O. ENGLER[1]; F. Friedel[2]; [1]Los Alamos National Laboratory, Center for Materials Science, Mail Stop K765, Los Alamos, NM USA; [2]Thyssen Steel Germany

The magnetic properties of Fe-3%Si electrical steel sheets for electrical transformers are mainly determined by their crystallographic textures. In most applications a texture with a preferred {011}<100>-orientation, called Goss-orientation, forms by discontinuous growth of Goss-oriented grains which pre-exist in the primary recrystallization texture, i.e., by secondary recrystallization. In the literature, there is a variety of approaches to correlate the preference of the Goss-orientation to its preference of so-called special or coincidence-site-lattice (CSL or low-S) grain boundaries. The present paper discusses an alternative approach to explain the dominance of the Goss-orientation, which is based on the concept of 'orientation pinning': Rather than assuming that certain grains are favored by a special orientation relationship, it is considered that growth of grains with some orientation relationships is disfavored. It is generally known that low-angle grain boundaries with misorientation angles below 15-20 degrees (Si) as well as coherent twin grain boundaries (S3) are characterized by a very low mobility. Thus, if upon secondary recrystallization a growing grain meets other grains with a similar or twin orientation, immobile grain boundary segments result which will act as obstacles to the moving grain boundary and, consequently, will pin it. Thus, in the long run, grains which are distinguished by a low probability of being pinned by creating immobile grain boundaries are preferred and would eventually predominate in the final texture.

12:00 PM LUNCH

Abnormal Grain Growth

Tuesday AM
June 16, 1998

Room: Rangos Hall-Room 3 (2nd floor)
Location: University Center

8:30 AM INVITED PAPER

ORIENTATION PINNING DURING GROWTH: D. JUUL-JENSEN[1]; [1]Riso National Lab, Materials Department, Roskilde DJ-4000 Denmark

The mobility of a grain boundary depend on the misorientation across the boundary. It is generally accepted that the mobility of low angle boundaries is low. Therefore, if a grain during its growth meets surrounding material with an almost identical crystallographic orientation, a low angle grain boundary or a low angle boundary segment is created which will move only slowly compared to high angle grain boundaries or high angle grain boundary segments. This retardation of growth, which has been termed "orientation pinning" [1], can have significant effects on the textural and microstructural development as well as on the growth kinetics. In the present paper the orientation pinning mechanism during recrystallization and grain growth processes is discussed. In the first section the mechanism is described and a brief overview of experimental rate results are given. In the next section, a Monte Carlo modelling approach is presented which allows orientation pinning to be simulated and results of both recrystallization and grain growth simulations are presented. In the final section of the paper, a new experimental tool - a 3D x-ray microscope - based on high energy synchrotron radiation is described. The instrument is presently under development at the European Synchrotron Radiation Facility (ESRF) in France, and an up-to-date status will be given. Finally, the potentials of this instrument for in-situ studies of growth of a selected single grain in the bulk of a larger sample, and thus the potentials for direct observations of orientation pinning, are discussed.

9:10 AM INVITED PAPER

MONTE-CARLO SIMULATION ON THE ABNORMAL GROWTH OF GOSS GRAINS IN Fe-3%Si CONVENTIONAL STEEL: J. A. SZPUNAR[1]; N. Rajmohan[1]; Y. Hayakawa[2]; [1]McGill University, Department of Mining and Metallurgical Engineering, Montreal, Quebec H3A 2B2 Canada; [2]Kawasaki Steel Corporation, Technical Research Laboratories, 1-Kawasakidouri, Mizushima, Kurashiki, Okayama 712 Japan

Goss texture development in Fe-3%Si conventional steel is investigated using a three-dimensional Monte-Carlo model incorporating a full description of the microstructure and crystallographic texture. The computer specimen composes of voronoi polyhedra which are descretized into lattice sites with three-dimensional honeycomb structure having 12 nearest neighbours. The experimental Orientation Distribution Function (ODF) is mapped on to the computer specimen by assuming random correlation between the adjacent grains. The simulations makes use of the experimental data on anisotropic grain boundary energy and calculated inherent mobility. Rapid coarsening of precipitate particles releases high energy boundaries at the early stages of annealing which is responsible for the development of Goss texture. This is identified by employing the concept of Oswald ripening and Zener pinning. The complex interaction between the particle coarsening and grain boundary migration is addressed. The result of the simulation is compared with experimental observations.

9:50 AM INTERACTIVE SESSION

11:20 AM

GRAIN BOUNDARY FACETING AND ABNORMAL GRAIN GROWTH IN NICKEL AND NICKEL ALLOYS: SUNG BO LEE[1];

Nong Moon Hwang[1]; Duk Yong Yoon[1]; [1]Korea Res Inst. of Standards & Science, Doryong-dong 1, Yusung-gu, Daejon 305-606 Korea

During the annealing of deformed Ni and Ni alloys, the occurrence of abnormal grain growth (AGG) and grain boundary faceting depends on the annealing temperature and carbon concentration. When deformed Ni specimens are annealed in vacuum, AGG occurs at all temperatures even close to the melting point, T_m. If Ni is carburized, AGG occurs at temperatures below $O.7T_m$ and normal grain growth (NGG) occurs above $O.7T_m$. In a model Ni-base alloy, AGG occurs when annealed at 1200ŸC but NGG at 1300ŸC. Whenever NGG occurs, all of the grain boundaries are smoothly curved, indicating disordered structures. Whenever AGG occurs, all or most of the grain boundaries are faceted, indicating that at least some of the boundaries have ordered structures. The results thus show that the occurrence of AGG depends on the grain boundary structure. These observations are consistent with the simulations which show that AGG stems from grain boundary anisotropy. The observations are also consistent with the possibility that AGG occurs from the peculiar migration kinetics of the ordered boundaries.

11:40 AM

EFFECT OF INTERNAL STRESSES IN DEFORMED BCC METALS ON THE ORIENTATIONS OF NEW GRAINS: Y. B. PARK[1]; L. Kestens[2]; J. J. Jonas[3]; [1]Sunchon National University, Department of Materials Science and Metallurgical Engineering, Sunchon 540-742 Korea; [2]Centrum voor Research in de Metallurgie, Department of Flat Rolling, Technologiepark 9, Gent B-9052 Belgium; [3]McGill University, Department of Metallurgical Engineering, Montreal, Quebec H3A 2B2 Canada

The internal residual stresses in a deformed matrix are evaluated on the basis of the slip systems that are active and the geometrically necessary dislocations. The orientations of the recrystallized grains that are expected to grow in the internally stressed matrix are predicted by means of a new recrystallization model. The model relies on two principles: first, the maximum principal stress direction in the deformed grain becomes the minimum Young's modulus direction in the recrystallized grain; second, a {110} plane within which the maximum principal stress direction (and hence. the minimum Young's modulus direction) lies, is taken as an invariant plane. The predictions obtained in this way are compared with experimental results and discussed in terms of the effect of internal stress on the textures produced in cold rolled as well as wire drawn bcc metals (steel, molybdenum, tantalum, tungsten, etc.).

12:00 PM LUNCH

TUESDAY PM

Triple Junctions

Tuesday PM — Room: Rangos Hall-Room 1 (2nd floor)
June 16, 1998 — Location: University Center

1:30 PM INVITED PAPER

2- AND 3-D CURVATURE DRIVEN VERTEX SIMULATIONS OF GRAIN GROWTH: C. MAURICE[1]; [1]Ecole Nationale Superieure des Mines de St. Etinnee (ENSMSE), Materials Dept., 42023 St. Etienne, Cedex 02 France

The orientation and temperature dependence of cellular structure growth is numerically simulated in both two and three dimensions by means of a vertex model. In this particular version of the model the motion of the vertices is governed by the grain boundary motion, which in turn, depends explicitly upon the local boundary curvature. The present work has concentrated on using real scale parameters with SI units in the simulation lengths are in metres, time in seconds, temperature in Kelvin, boundary energy in $J.m^2$ and boundary mobility in $m^4.J^{-1}$. Realistic microstructures are described by polygonal shaped grains having crystallographic orientations given by three Euler angles. Knowing the orientation of two adjacent grains, the grain boundary character is easily determined the grain boundary energy and mobility can therefore be misorientation dependent. Finally the annealing temperature is introduced via the thermal activation of the grain boundary mobility. Several case studies (mostly 2D) of microstructural instability are presented to illustrate the versatility of the simulation. Ideal normal grain growth with isotropic interfaces is shown to closely reproduce soap froth experimental results. The effect of misorientation dependent boundary energies and mobilities is investigated, with particular emphasis on microstructures featuring orientation and/or grain size gradients.

2:10 PM

ATOMISTIC SIMULATIONS OF GRAIN BOUNDARY TRIJUNCTIONS: S. G. SRINIVASAN[1]; John W. Cahn[1]; Hannes Jonsson[1]; Gretchen Kalonji[1]; [1]University of Washington, Department of Materials Science and Engineering, Seattle, WA 98195-2120 USA

The role of grain boundary junctions in grain growth process has received little attention. The excess free energy of the common line of intersection of the three crystalline interfaces, the trijunction lines, must be a factor in the evolution of junction morphology and grain switching rearrangements that are part of the grain growth process; under certain conditions it is conceivable that this energy could arrest grain growth. We report results of an atomistic molecular dynamics simulations of a periodic three-dimensional Lennard-Jones system consisting of three FCC grains rotated 30 degrees about a common <001> axis. This configuration yields six trijunctions, also along <001>, and their associated symmetric tilt grain boundaries. An aluminum specimen with such grains was manufactured and studied using high-resolution electron microscopy by Dahmen and co-workers. They found highly symmetric trijunctions that were later classified by Cahn and Kalonji as alternating among two symmetry classes. Our simulations of such a system address the following basic questions: (i) which classes of trijunctions occur, (ii) what is the atomic structure in the vicinity of the trijunctions, (iii) what are their energies, and (iv) how does the structure and energy of our system vary as a function of grain size.

2:30 PM

BOUNDARY AND JUNCTION MOBILITIES AND MIGRATION MECHANISMS: MONEESH UPMANYU[1]; David J. Srolovitz[1]; Lasar S. Shvindlerman[2]; [1]University of Michigan, Materials Science and Engineering, 2300 Hayward, H. H. Dow Building, Ann Arbor, MI 48109 USA; [2]Institute of Solid State Physics, Russian Academy of Sciences, 142432, Chernogolovka, Moscow District RUSSIA

We present results of molecular dynamics simulations of the curvature driven grain boundary migration. Following the work of Shvindlerman and co-workers, two distinct simulation geometries are examined: a U-shaped half-loop bicrystal (for constant driving force studies and a straight, symmetric tilt boundary intersecting a half-loop grain at its apex (for junction migration studies). Examination of half-loop shrinkage rates for different half-loop widths show that grain boundary velocity is proportional to boundary curvature, in agreement with existing theories. Next, we demonstrate that the boundary mobility is an Arrhenius function of temperature. Examination of the atomistic mechanisms of grain boundary migration show that while well-defined atomic hops across the boundary do occur, it is the sudden, correlated motion of much larger groups of atoms that dominate the (high) curvature driven grain boundary migration process. Boundaries with high symmetry misorientations migrate faster than and by correlated jumps of larger groups than do general boundaries Junction migration studies demonstrate that the dynamic triple junction angle is the same as that found in static simulations. Measurements of the triple junction mobility will be presented and its influence on curvature driven growth discussed.

2:50 PM INTERACTIVE SESSION

3:50 PM INVITED PAPER

MOTION OF TRIPLE JUNCTIONS: A MATHEMATICAL STUDY: F. REITICH[1]; [1]University of Minnesota, Department of Mathematics, Minneapolis, MN 55455 USA

The objective of this presentation is to introduce some fairly novel mathematical ideas (such as level set formulations and viscosity solutions) that have proven useful in the mathematical analysis (both theoretical and numerical) of interfacial dynamics. For definiteness, we will concentrate on the motion of triple junctions in polycrystalline materials. We shall represent these with a classical geometric model whereby ideal grain boundaries advance to minimize surface and bulk energies. We will show how a careful mathematical analysis can lead, for instance, to a qualitative understanding of the motion of trijunctions in the (singular) case of small surface energies. The issues that arise in the search for effective algorithms for computer simulations will also be addressed.

4:30 PM

EQUILIBRIUM AT TRIPLE JUNCTIONS UNDER THE INFLUENCE OF ANTISOTROPIC GRAIN BOUNDARY ENERGY: ALEXANDER H. KING[1]; [1]State University of New York at Stony Brook, Department of Materials Science & Engineering, Stony Brook, NY 11794-2275 USA

We study the conditions required of equilibrium configurations at triple junctions, under the influence of grain boundary energy that can vary with boundary inclination, through application of the Hoffman-Cahn capillary vector. It is shown that relatively simple geometric constructions can be used, which are analogous to the usual force-triangle method used under isotropic conditions. Particular attention is paid to cases in which one, two or three of the boundaries are trapped in orientations that are associated with energy cusps, and it is shown that these are often able to accommodate wide variations of grain boundary energy and/or inclination. Some cases generate "bi-stable" configurations in which one or two of the boundaries can flip between different stable inclinations. The case of a twin boundary meeting an isotropic grain boundary is analyzed in detail, and shown to produce some unique solutions for the inclination of the grain boundary relative to the twins. Cases of triple junction pinning will be described, and the principles of their influence upon the equilibrium configurations will be explained semi-quantitatively.

4:50 PM

THE EFFECTS OF GRAIN BOUNDARY LIQUIDATION ON GRAIN GROWTH: ANDRE LAMONT WILSON[1]; Paul R Howell[1]; Richard Peter Martukanitz[2]; [1]The Pennsylvania State University, Metals Science and Engineering, 209 Steidle, University Park, PA 16802 USA; [2]Applied Research Laboratory, High Energy Processing, P.O. Box 30, State College, Pennsylvania 16801 USA

The liquidation of grain boundaries in the heat-affected zone during welding and other high heat input processes and its effect on normal grain growth has been investigated through experiment and computer simulation. During a typical welding procedure as normal grain growth occurs in the HAZ, the migrating grain boundaries either encounter the liquidated particles and are subsequently wetted by the liquid phase or they sweep up segregants from the matrix which are then liquidated at the boundaries. Grain boundary liquidation has been found to hinder grain growth in laser clad microalloyed and non-microalloyed steels. Measurements of the grain growth kinetics of commercial and laboratory steels have been made after isothermal heat treatments, weld simulations, and arc welding procedures. These experiments were then "duplicated" on a computer utilizing a Monte Carlo algorithm for simulating curvature-driven grain growth. The algorithm can successfully reproduce the isothermal grain growth kinetics observed in the steels without microalloy additions. The algorithm also generates grain structures that are comparable with actual steel weld heat-affected zones when an appropriate temperature gradient is applied. The effects of thermal pinning and grain boundary liquidation pinning are examined.

5:10 PM ADJOURN

Grain Growth Models

Tuesday PM
June 16, 1998

Room: Rangos Hall-Room 3 (2nd floor)
Location: University Center

1:30 PM INVITED PAPER

USE OF SURFACE EVOLVER IN THE SIMULATION OF GRAIN GROWTH AND SUBGRAIN GROWTH: KNUT MARTHINSEN[1]; Ola Hunderi[2]; Nils Ryum[3]; [1]SINTEF, Materials Technology, Trondheim N-7034 Norway; [2]Norwegian University of Science and Technology, Physics, Trondheim N-7034 Norway; [3]Norwegian University of Science and Technology, Metallurgy, Trondheim N-7034 Norway

In spite of its technological importance and the fact that grain growth has been extensively studied for many decades, far from all fundamental aspects of grain growth are yet fully understood. In the present work the program Surface Evolver has been used to simulate normal grain growth as well as subgrain growth in two dimensions. Surface Evolver is an interactive computer program that minimizes the energy of a surface subject to constraints. The energy can include surface energy, gravity and other forms. The minimization is done by evolving the system towards a minimal total surface energy by a gradient descent method. The essential difference between normal grain growth and subgrain growth relates to the difference in mobility between the grain boundaries and the triple lines. The effect is that while normal grain growth takes place with grain boundaries having a uniform curvature (as part of a sphere), subgrain growth is assumed to take place with approximately planar grain boundaries (in 3D). The presentation will focus on grain growth kinetics, the grain size distribution functions and spatial grain size correlations and discuss possible differences in the two cases. Some aspects of abnormal grain growth will also be discussed and also grain growth in the presence of an isotropic and homogeneous Zener drag.

2:10 PM

SIMULATION OF RECRYSTALLIZATION USING A 3D CELLULAR AUTOMATION APPROACH: VOLKER MARX[1]; Günter G. Gottstein[1]; [1]RWTH Aachen, Institut für Metallkunde und Metallphysik, Kopernikusstr.14, Aachen D-52056 Germany

A 3D model has been developed to simulate both primary static recystallization and recovery of cold worked metals. The model is based on a modified cellular automaton approach and incorporates the influence of crystallographic texture and microstructure in respect to both mechanisms mentioned above. The model takes into account nucleation and the subsequent growth of the nuclei. It is possible to vary the kinetics of nucleation, e.g. site saturated or constant nucleation rate. Subsequent growth of the nuclei terminates upon impingement. The local growth rate of the nuclei is determined by the local stored energy of the deformed matrix (i.e. the driving pressure) and the misorientation between a growing nucleus and its surrounding matrix (i.e. the grain boundary mobility). This approach allows to introduce different conditions for recovery, nucleation and grain growth. The model simulates kinetics, microstructure and texture development during heat treatment discrete in time and space.

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APPLICATION OF A 3D STOCHASTIC CELLULAR AUTOMATION FOR THE DISCRETE MESOSCALE SIMULATION OF GRAIN GROWTH PHENOMENA: D. RAABE[1]; [1]Carnegie Mellon University, Department of Materials Science and Engineering, Pittsburgh, PA 15213-3890 USA

The paper introduces a 3D stochastic cellular automaton for the spatial kinetic and crystallographic simulation of mesoscale transformation phenomena that involve non-conserved structural field variables and the motion of sharp interfaces such as encountered in grain growth. The differential equation that acts as a local transformation rule consists of the probabilistic form of a classical linear symmetric rate equation for grain boundary segment motion. All coupled differen-

tial equations of motion are simultaneously solved using a weighted stochastic sampling integration scheme. The method is much faster than conventional finite difference methods. The automaton is discrete in time, real space, and orientation space. The paper shall discuss var-ious 3D examples.

2:50 PM INTERACTIVE SESSION

3:50 PM INVITED PAPER

MODELING OF NUCLEATION DURING RECRYSTALLIZATION: B. RADHAKRISHNAN[1]; [1]ORNL, Materials and Ceramics Division, Oak Ridge, TN 37831-6140 USA

The dislocation substructure of a deformed material is known to consist of subgrain networks. Regions of high stored energy are characterzed by small subgrains and a large misorientation between the subgrains. Nucleation during recrystallization is known to occur by the heterogeneous growth of subgrains at these locations. The formation of a high angle boundary associated with a recrystallized nucleus is favored by the presence of long range orientation gradients in the cold worked microstructure. The paper discusses the development arid application of a Monte Carlo grain growth algorithm for simulating the abnormal growth of subgrains. The microstructural requirements for abnormal grain growth and formation of recrystallization nuclei are examined by systematically varying the magnitude and range of the orientation gradient and observing their influence on the kinetics of subgrain growth. The subgrain growth algorithm is then implemented in a realistic three-dimensional microstructure deformed in plane strain compression. The stored energy of deformation and the orientation of sites in the deformed microstructure are obtained by a finite element technique based on crystal plasticity approach. The application of the Monte Carlo subgrain growth algorithm to the deformed microstructure results in the prediction of the orientation as well as the spatial distribution of the recrystallized nuclei as a function of the extent of prior cold work.

4:30 PM

PHASE-FIELD SIMULATION OF GRAIN GROWTH: L. Q. CHEN[1]; [1]Pennsylvania State University, Department of Materials Science and Engineering, University Park, PA 16802 USA

A grain growth simulation model based on a diffuse-interface description of grain boundaries will be described. In this model, grain orientations are represented by a multiple-component non-conserved order parameter whose temporal evolution is governed by systems of time-dependent Ginzburg-Landau equations. With the input of initial microstructure and necessary parameters for specifying the grain boundary energy and mobility, it produces microstructural evolution automatically without tracking the positions of grain boundaries. Results on grain growth kinetics in both two- and three-dimensions will be presented, and compared to those obtained using other simulation models and analytical theories. Its applications to more complicated grain growth phenomena such as grain growth with solute-drag, and coupled grain growth and Ostwald ripening will be discussed.

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GRAIN GROWTH SIMULATION: A NEW MODEL: P. PAILLARD[1]; [1]ISITEM, Laboratoire de Génie des Matériaux, Rue Christian Pauc, BP 90604, Nantes, Cedex 44306 03 France

Recrystallization is one among phenomena of fundamental importance in materials engineering. However, due to the collective behavior of interfaces during grain growth and the difficulties inherent to its analytical description, computer simulation has revealed being a unique tool capable of a statistical treatment of the microstructural evolution during annealing. In this paper, a new simulation method of grain growth is presented which overcomes well known limitations of existing approaches and offers remarkable description capabilities of several experimental situations among which primary recrystallization, Zener drag effects and evolution features of an initially heterogeneous microstructure. The limitations of Monte Carlo and Vertex techniques are briefly discussed while compared to the solutions adopted by this new technique. The validation of the latter has been obtained by generic, two-dimensional simulations of grain growth. The results of which are briefly presented together with perspectives for future work.

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MODELLING OF PRIMARY RECRYSTALLIZATION IN STAINLESS STEELS: I. SALVATORI[1]; G. Abbruzzese[1]; [1]CSM Terni Unit, Terni I-051000 Italy

A mathematical model, able to describe the primary recrystallization of stainless steels has been developed. This model concerns the evolution of deformation cells (subgrains) in grains, by applying the concepts of the grain growth statistical model. It supposes that the recrystallization nuclei are present in the deformed matrix of the metal as areas relatively free from dislocations, and they are statistically represented by their size distribution. When a deformed material is subjected to heat treatment, the movement of subgrain boundaries is activated. Such boundaries delimit the areas free from dislocations (relatively low angle grain boundary), and the subgrain growth in the deformed matrix (driving force χ dislocation density difference) occurs against the boundary energy generated by the crystals misorientation. The grains, at first assumed all activated at the same time, freely grow in the deformed matrix until they get in contact each other, by means of a continuous passage from the growth activated by deformation gradient to a proper grain growth process activated by only grain boundary energy. This model, in its simplified version, allows to reproduce the role of incubation phenomena and relates it to the type of the initial distribution. Moreover it describes the continuous change of kinetics, from Avrami to grain growth type. Moreover it is also possible to describe the effect on the recrystallization microstructure of the heating rate during annealing. Results from the model are here discussed in comparison with available experimental data on BCC-iron and measurement performed on stainless steels. By this model it is possible to analyze the role of recovery process on the kinetics and on the generated recrystallized microstructure. Finally, in this framework, it is relatively easy to perform the extension of the model to include texture and drag effects.

5:30 PM ADJOURN

8:00 PM
Workshop on Simulation Methods for Grain Growth, D. J. Srolovitz, Discussion Leader

Tuesday PM
June 16, 1998

Room: Rangos Hall-Room 1 (2nd floor)
Location: University Center

WEDNESDAY AM

Particles

Wednesday AM
June 17, 1998

Room: Rangos Hall-Room 1 (2nd floor)
Location: University Center

8:30 AM INVITED PAPER

EVOLUTION OF GRAINS AND PARTICLES IN MICROSTRUCTURE: M. E. GLICKSMAN[1]; [1]Rensselaer Polytechnic Institute, Troy, NY 12180-3590 USA

Recent studies conducted in our laboratory on a high-purity model system show that the normal evolution of two-dimensional polycrys-

tals follow predictions of the Mullins-von Neumann kinetic law for individual grains. Mullins-von Neumann kinetics assume uniform boundary behavior (constant boundary energy and mobility), vertex equilibrium, and flow by mean curvature. Although individual grains in the polycrystal are observed to exhibit growth and shrinkage rates that differ substantially from theories like Mullins-von Neumann, each topologically segregated sub-population of grains tends to obey this law on average. Precipitate evolution models will also be reviewed, and progress on identifying the physical length scales entering the late-stage phase coarsening kinetics will be discussed. We find that in simulated microstructures containing a finite number of interacting precipitates, two length scales may be identified at low volume fractions: 1) the mean-free interparticle spacing and 2) the diffusional Debye length. Providing the system is not too sparse, the Debye length is rate controlling, and provides an evolution rate that increases with the square-root of the volume fraction. In extremely sparse systems, the interparticle spacing becomes rate controlling, and provides an evolution rate that increases with the cube-root of the volume fraction.

9:10 AM

GRAIN GROWTH IN CONTINUOUSLY RECRYSTALLIZED ALUMINUM WITH FINE DISPERSED PARTICLES: Fumie Seki[1]; Jian Li[2]; S. SAIMOTO[2]; K. Itoh[1]; T. Kamijo[3]; [1]University of Tokyo, Department of Materials Science, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113 Japan; [2]Queen's University at Kingston, Kingtston K7L 3N6 Canada; [3]Yokohama National University, Dept. of Mechanical Eng., 156 Tokiwadai, Hodogayu-ku, Yokohama 240 Japan

The classical model of time-dependent grain growth by Burke and Turnbull (BT) whereby the grain radius R(t) is proportional to t˚ has not been readily observed. The reasons for this situation is attributed to the fact that in the real material other factors pre-empt the grain boundary energy (γ) as driving force (γR) especially since discontinuous recrystallization results in large equiaxed grains. On the other hand during continuous recrystallization we have found that the equiaxed grains can be an order of magnitude smaller in the 1-2 um range. Grain growth of these grains at 240ϒC takes place in accordance with the BT model but at 270ϒC, discontinuous growth sets in. The texture retains the as-deformed one during uniform growth with only detectable amounts of the cube component. Only during discontinuous growth does the cube texture become prominent and this is verified by electron back scattered diffraction examination of the largest growing grains. In this study the success of the thermal mechanical process required to produce continuous recrystallization will be shown to be the role of Fe solutes On the other hand the role of the $FeAl_3$ dispersoids can be manifested by a limiting grain size at 240ϒC. Thus distinct separation of the grain growth mechanisms has been achieved.

9:30 AM

MEASUREMENTS OF GRAIN BOUNDARY MOBILITY IN ALUMINIUM BY IN-SITU SEM EXPERIMENTS: Y. HUANG[1]; F. J. Humphreys[1]; [1]Manchester Materials Science Centre, Grosvenor Street, Manchester M1 7HS England

Previous work has shown combined in situ annealing and EBSD in an SEM to be a rapid and powerful method of studying annealing, and the present paper presents a systematic study of the mobility of high angle grain boundaries under conditions of driving pressure which are relevant to recrystallization. Small (3x3xlmm) samples from plastically deformed single crystals or large grained polycrystals of a single-phase A1-O.O5wt%Si alloy have been isothermally annealed at temperatures between 230ϒC and 320ϒC in an SEM. Recrystallization was induced at a scratch on the sample surface, and the evolution of microstructure as imaged using backscattered electrons, was recorded by standard and video methods so that boundary velocities could be determined. The subgrain structures prior to and after annealing were determined by EBSD and from this the subgrain sizes and misorientations and hence the driving pressure for recrystallization were determined. The boundary velocities were found to be proportional to the driving pressure, and the mobilities were thus determined. Temperature dependence of the mobilities indicated an activation energy similar to that for self diffusion in aluminium. The orientation dependence of boundary mobility was measured and the results are compared with previous work.

9:50 AM

APPLICATION OF POWDER ENGINEERING: A WAY TO CONTROLLED FORMATION OF CERAMICS MICROSTRUCTURE: V.V. ISCHENKO[1]; O.A. Shlyakhtin[1]; N.N. Oleinikov[1]; Yu. D. Tretyakov[1]; [1]Moscow State University, Chemistry Dept., Inorganic Chemistry Div., Moscow 119899 Russia

There is an evident correlation between precursor's and product's microstructures. The path the microstructure evolution follows during thermal or other kinds of sample's treatment is essentiallydependent not only on the conditions of the treatment but also on microstructure of the preceding compounds. Grain growth in BaZrO3 powders was studied upon their annealing in temperature range 700-1300C. The correlation among initial microstructure of salt precursor mixture prepared by freeze-drying technique, oxide powder's microstructure obtained upon thermal decomposition and its evolution during following ceramics preparation procedures was found out. Based on aggregate structure considerations, a new approach formicrostructure modification was proposed. Ultrasonic treatment applied at different stages of powders processing enabledthe evolution of microstructure (in particular, the character of grain growth) to be considerably changed. The process of densification of differently prepared BaZrO3 ceramics was also studied. The dependencies of relative densitieson aggregate size distribution and its relation with grain growthin ceramics being sintered at 1600 C were investigated.

10:10 AM BREAK

10:30 AM

THE GRAIN GROWTH IN STRUCTURAL STEELS: DEPENDENCE ON ALLOYING ELEMENTS AND THEIR COMBINATION: BERTOLD B. VINOKUR[1]; Oleg G. Kasatkin[2]; [1]Doctor of Normal and Abnormal Grain Growth, 3901 Conshohocken Ave., Apt. E-21, Philadelphia, PA 19131 USA; [2]E.O. Paton Institute of Electrical Welding of National Ukrainian Academy of Science, 11Bozhenko St., Kiev 252005 Ukraine

The grain growth of austenite in structural steels depends on the nature of alloying elements, their surface energy, surface tension, carbide-forming ability, dissolution temperature of carbides, et al. In the absence of previous investigations, the influence of all alloying elements and their combinations on the austenite grain growth under identical conditions was studied. Such experiments were carried out with more than 100 steels that have absolutely the same metallurgical history. The well-known G. Hanemann's method was used to obtain the stability of austenite grain size in the temperature range 800 to 1400ϒC. It was analyzed, and estimated the possibility of using different empirical models (including the Arrenius' equation) to describe grain growth. It was found that only a model using Taylor's series (with 3 terms) can really reflect the grain growth processes. Quantitative estimate of the influence of each alloying element and their combination was carried out with multiple regression analysis. The resultant models were transformed, such that the grain growth can be described depending on Ac3 critical point temperatures. This allows one to calculate the coefficients of polynomial of Taylor's series (i.e., interpolation regression models). For this, the interpolation model-dependence point Ac3 on alloying elements and their combinations also were obtained using more than 800 literature data. Analysis of all obtained models of the grain growth and the Ac3 critical point show that the models work very well: this is corroborated in comparison with experimental and calculated data. All programs for calculation are available in the E.O. Paton Scientific Research Institute of Electrical Welding.

10:50 AM

GRAIN REFINEMENT AND GROWTH BY MECHANICAL ATTRITION: H. H. TIAN[1]; M. Atzmon[2]; [1]University of Michigan, Department of Materials Science and Engineering, 99, Ann Arbor, MI 48109 USA; [2]University of Michigan, Department of Nuclear Engineering and Radiological Sciences

Mechanical attrition has been known to produce nanocrystalline powders of elemental metals and alloys. Although the properties of

nanocrystals have been studied in detail, the mechanisms of their formation have not been determined conclusively. In particular, researchers have been seeking to identify the factors that determine the lowest grain size. A number of authors have suggested a competition between grain refinement arid thermally activated processes. In an effort to understand the process of grain refinement by mechanical attrition, we have studied the evolution of grain size and RMS strain in Fe as a function of time during low-energy ball milling. Over 140 data points were obtained for different milling intensities arid temperatures. Warren-Averbach analysis of x-ray data was used to determine the grain size and RMS strain, and the contribution due to stacking faults was observed to be negligible. We find that above a grain size of D=15 nm, $D^{\alpha t \cdot 12}$ with little temperature dependence. Below 15 nm, the evolution law changes and a temperature-dependent steady state is reached. In this paper, the experimental results will be compared with available models. Further, measurement results of grain growth kinetics will be presented for samples formed at different temperatures. These will be compared with recent measurements in nanocrystals formed by high-energy ball milling, which were found to display transient grain growth at anomalously low temperatures.

11:10 AM

INFLUENCE OF MELT PROCESSING TREATMENT ON THE LARGE CRYSTALLINE YBCO CERAMICS FORMATION: DENIS IGOREVICH GRIGORASHEV[1]; Ann Petrovna Soloshenko[1]; Nickolay Nickolaevich Oleynikov[1]; [1]Moscow State University, Dept. of Chemistry, Inorganic Chemistry, V-234 Lenin Hills, Moscow 119899 Russia

In this work the processes of large-crystalline YBa2Cu3Oz-based superconducting ceramics formation by melt processing techniques were studied. There was investigated the influence of the parameters of melt treatment on the grain growth and orientation. It was found to be possible to increase significantly grain size when apply very slow cooling rates of the melt and use of seeding crystals. From another hand it is very important to control thoroughly temperature of slow cooling step starting because of possibility for growing crystals to change their orientation. After the optimization of all steps of the heat treatment ceramic samples with the grain size about 10 mm were obtained. Finally, there were made some conclusions about the infuence of processing parameters on the microstructure formation and superconducting properties of samples.

11:30 AM ADJOURN

Steels-1

Wednesday AM Room: Rangos Hall-Room 3 (2nd floor)
June 17, 1998 Location: University Center

8:30 AM INVITED PAPER

STABILITY AND GROWTH OF GRAIN AND STRUCTURES IN TWO-PHASE MATERIALS: E. J. HUMPHREYS[1]; [1]UMIST (University of Manchester), Metallurgy & Materials Science Department, Manchester M60 1QD UK

A new analytical model of the stability and growth of cellular microstructures such as subgrain and grain structures has recently been presented. The theory is based on an analysis of the stability of cellular microstructures in which the energy and mobility of the cell boundaries are variables. Although the level of this approach is somewhat simpler than many recent theories of recovery recrystallization and grain growth, such an analysis has the advantage that not only is it simple and transparent, but that it treats all of these phenomena in a unified manner, enabling the analysis of processes which do not readily fall into any of the three traditional categories. In addition, the effects of important materials variables such as texture and second-phase particles are readily incorporated into the theory. The paper will discuss the application of the theory to the recovery, recrystallization and grain growth of particle-containing materials, consider the refinements which are required for materials in which the particles are not stable, and the results will be compared with those from existing, more specialized theories models and simulations.

9:10 AM

COMPETITION BETWEEN RECOVERY AND RECRYSTALLIZATION DURING ANNEALING OF IF-STEELS: S. L. Lanteri[1]; H. Petigand[1]; H. RÉGLÉ[1]; [1]IRSID, Central Research Lab. USINOR Physical Metallurgy Dept., Voie Romaine - BP 30320, Maizières-lès-Metz 30320 France

Interstitial free steels used in automotive applications are typically hot- and cold-rolled and then continuously annealed. The recrystallisation texture developed during annealing will control the sheet's forming properties. In order to be able to accurately predict the recrystallisation kinetics and textures, we need to clarify which mechanisms are involved during annealing. Several studies have already shown that the nucleation step is of prime importance in recrystallisation texture formation. This stage in the process is, however, not completely understood. In this paper, we analyse the effect of a prior recovery treatment on the subsequent recrystallisation behaviour of a deformed steel, using either warm-rolled, or cold-rolled and recovered, samples as starting materials. The particularity of warm-rolling is the development of a deformation sub-structure which is almost completely recovered. The stored energy is thus essentially concentrated in interfaces and the driving force for boundary migration is interface area reduction. Nucleation can be considered as abnormal sub-grain coarsening, and recrystallisation will take place without requiring additional recovery. The cold-rolled specimen has a blurred deformation substructure consisting of cells with high dislocation densities. Here, the boundary migration is driven by both the dislocation density gradient and interface area reduction. The nucleus development stage will still need some recovery to rearrange tangled dislocation walls into mobile interfaces. A prior recovery heat-treatment on this sample was found surprisingly to accelerate the subsequent recrystallisation kinetics.

9:30 AM

A MECHANISM OF GOSS TEXTURE DEVELOPMENT IN SECONDARY RECRYSTALLIZATION IN ELECTRICAL STEEL: M. KUROSAWA; Y. Hayakawa; M. Komatsubara; J.A. Szpunar; Kawasaki Steel Corporation; Technical Research Laboratories; Kawasakidori 1-choe, Kurashiki-City, Mizushima, 712 Japan

A mechanism of Goss texture development during the secondary recrystallization in Grain-oriented electrical steel is proposed based on the physical properties of the high-energy boundaries. From the analysis of the primary recrystallized texture, the frequency of the high-energy boundaries is proved to be the highest around the Goss grain. The high-energy boundary has more structural defects, which are linked to a high mobility and a high grain boundary diffusion rate. Quicker coarsening of precipitates enables high-energy boundaries to move earlier than other boundaries during final annealing. Thus, the Goss grain has a growth advantage of having the highest number of mobile boundaries during the progress of final annealing. In order to verify the proposed model of secondary recrystallization, Monte-Carlo simulation and the investigation of the grain boundary character distribution were performed, and both simulated and experimental results supported the assumption which is used in this model.

9:50 AM

CUBE TEXTURE FORMATION IN COLD ROLLED AND ANNEALED ULTRA LOW CARBON STEELS: LEO KESTENS[1]; J. -C. Herman[1]; V. Leroy[1]; [1]Center for Research in Metallurgy, Flat Rolling Department, Technologiepark 9, Gent B-9052 Belgium

In a cold rolling and annealing experiment applied to an ultra low carbon steel (with a carbon content of 0.002 mass% in solid solution) it was observed that the cube component appears as a minor or secondary peak in the recrystallization texture after cold rolling and annealing. The intensity of these cube components increases with larger rolling reductions. Showing a pronounced effect of orientation selectivity the cube components gradually disappear during normal grain growth after

primary recrystallization. The origin of the cube component in the primary recrystallization texture was investigated by local orientation measurements on partially recrystallized structures at the very early stages of recrystallization. These measurements revealed a very high orientation spread in the substructure of {111} deformed bands, locally showing subgrains with near cube orientations. A microstructural analysis shows that these near cube subgrains give rise to a cube component in the nucleation texture, already in the very early stages of recrystallization. The present observations demonstrate that subgrain growth in the recovered microstructure triggers the onset of recrystallization. Subgrain growth is most likely to occur in these bands of the substructure with the highest local misorientation gradients and therefore cube oriented subgrains have an increased growth potential to consume the {111} oriented substructure of the surrounding matrix.

10:10 AM BREAK

10:30 AM

THE USE OF STABLE PARTICLES FOR THE PREVENTION OF GRAIN COARSENING IN THE HEAT AFFECTED ZONE OF STEEL WELDMENTS: REBECCA L. FAZACKERLEY[1]; [1]Microalloying International, Inc., 10175 Harwin, Suite 110, Houston, TX 77036 USA

Microalloying additions, niobium, vanadium and titanium, which form stable nitride and carbide particles, are frequently used in conjunction with aluminum nitride, to control the grain size of HSLA steels. The effectiveness of grain refinement is related to the stability of the different compounds at high temperatures which controls dissolution and particle coarsening kinetics. Titanium nitride can be used to inhibit austenite grain growth at temperatures up to 1250°C. However, due to demands for more effective control of grain size in the heat affected zone of steel welds at very high heat inputs, the need for particles which are stable at higher temperatures has arisen. Therefore, consideration has been given to oxide particles. Oxide particles are present in all steels but commonly the inclusion sizes are large and despite the quite large volume fraction they only inhibit the growth of extremely coarse grains. The presence of such large inclusions reflects both the oxygen contents and the restricted solubility of oxides in molten steel. However with careful control of steel composition, with regard to oxygen content and oxide forming element content, it is theoretically possible to control precipitation of oxide particles so that it occurs during solidification or in the solid steel. It has been shown, using powder metallurgy methods, that prevention of grain coarsening in the heat affected zone of welds, by the use of fine, stable particles is possible. It is expected that with careful control of steel composition it will be possible to prevent grain coarsening at high temperatures in conventionally produced steel. The present work has considered the precipitation and grain coarsening characteristics of SiO2 particles and compared the results with existing data for TiO2 and Al2O3 particles. It is concluded that for normal silicon and oxygen contents in concast steel, SiO2 alone does not offer practical potential as a high temperature grain refiner. The results have been rationalized in terms of the Gladman model. Suggestions for additional research are presented.

10:50 AM

THE EFFECT OF SUBCRITICAL ANNEALING ON AIN MORPHOLOGY AND ABNORMAL GRAIN GROWTH DURING SUBSEQUENT CARBURIZING OF COLD WORKED STEEL: KEITH C. EVANSON[1]; George Krauss[2]; [1]Colorado School of Mines, Metallurgical and Materials Engineering Dept., Hill Hall, Golden, CO 80401 USA; [2]Colorado School of Mines, Metallurgical and Materials Engineering Department., Hill Hall, Golden, Colorado 80401 USA

Abnormal austenite grain coarsening occurs during carburizing of conventionally produced aluminum-killed carburizing steels applied to cold forging applications. Laboratory heats of carburizing-grade 8720 steel with varied aluminum and nitrogen contents were processed to simulate conventional steel production including casting, bloom rolling and billet rolling prior to simulating cold-forging and carburizing. The soak temperature prior to the final rolling was varied along with the amount of cold-upsetting. By incorporating a subcritical annealing treatment after the final rolling stage but prior to the cold-upsetting, the abnormal austenite grain coarsening during carburizing was found to be significantly reduced for all combinations of chemistry and processing. Without the subcritical annealing treatment, abnormal grain coarsening is severe in all cases with some dependence on chemistry and processing. In subcritically-annealed specimens, the dependence of austenite grain coarsening on aluminum and nitrogen content and on soak temperature prior to final rolling is more pronounced. The pre-cold-work annealing treatment apparently serves to produce a beneficial distribution of AlN particles that effectively pin austenite grain boundaries during subsequent carburizing. AlN precipitation was examined using TEM extraction replicas. The austenite grain coarsening effects are discussed in terms of differences in AlN precipitation behavior, degree of local strain, austenite nucleation and growth behavior, and AlN evolution during carburizing.

11:10 AM

REAL-TIME MONITORING OF AUSTENITE GRAIN GROWTH IN STEEL USING LASER-ULTRASONICS: MARC DUBOIS[1]; Matthias Militzer[2]; Andre Moureau[1]; Jean F. Bussier[1]; [1]National Research Council Canada, Industrial Materials Institute, 75 Mortagne, Boucherville, Quebec JB4 6Y4 Canada; [2]University of British Columbia, The Centre for Metallurgical Process Engineering, Vancouver, British Columbia Canada

Laser-ultrasonics, a technique based on the generation of ultrasonic waves by a pulsed laser and on their detection by a laser interferometer, was used to monitor ultrasonic attenuation in steel at temperatures corresponding to hot rolling. In most metals, ultrasonic attenuation is mainly caused by scattering and is therefore sensitive to grain size. A calibration based on the metallographic evaluation of austenite grain sizes on quenched steel samples was obtained to relate quantitatively ultrasonic attenuation to austenite grain sizes. Employing this calibration, austenite grain growth was measured at temperatures up to 1200ϒC in a variety of steels, including an interstitial free steel for which austenite grain sizes cannot be determined by conventional metallographic techniques. An important advantage of this new technique is to provide an in-situ information with a time resolution that may be as low as 50 ms. Furthermore, the average microstructure over the whole thickness is measured and little or no sample preparation is required. The results presented in this paper show that laser-ultrasonics is a powerful laboratory tool to study microstructural evolution during hot rolling.

11:30 AM ADJOURN

WEDNESDAY PM

8:00 PM
Demonstrations of Simulation Methods and Discussion, Dierk Raabe, Discussion Leader

Wednesday PM
June 17, 1998

Room: Rangos Hall, Peter Room (2nd floor)
Location: University Center

8:00 PM
Poster Presentations

Wednesday PM
June 17, 1998

Room: Rangos Hall, Room 2 (2nd floor)
Location: University Center

THURSDAY AM

Thin Films

Thursday AM — Room: Rangos Hall-Room 1 (2nd floor)
June 18, 1998 — Location: University Center

8:30 AM INVITED PAPER

GRAIN GROWTH AND GRAIN SIZE DISTRIBUTIONS IN CONTINUOUS AND PATTERNED THIN FILMS: H. J. FROST[1]; [1]Dartmouth University, Thayer School of Engineering, Hanover, NH 03755 USA

Simulations of two-dimensional normal grain growth lead to a scaling state characterized by a grain size distribution with a specific time invariant shape, which is at least similar to that obtained for froths evolving between plates and to distributions predicted using mean field models which include topological transitions. However, thin films often are characterized by lognormally distributed grain sizes; in the as-deposited state, after 'normal' grain growth, and after abnormal grain growth. We have shown that front-tracking simulations which include drag effects due to surface grooves or solutes can lead to lognormal grain size distributions, and may explain some of the experimental observations. These simulations have been used to explore the statistical characteristics of the grain structures of patterned films, and to link these to the statistics of the reliability of patterned films. The effects of post-patterning grain structure evolution have also been investigated for a variety of patterned shapes.

9:10 AM

OBSERVATION OF PREFERRED GRAIN GROWTH IN ALUMINUM LINES: DAVID P. FIELD[1]; J. E. Sanchez[1]; H. Weiland[1]; [1]392 E. 12300 S. Suite H, Draper, UT 84020 USA

In-situ observation of grain growth in patterned aluminum lines was performed to track the evolution of texture strengthening during the post-patterning anneal. Specimens with line widths varying from 0.5 to 4 microns were analyzed using conventional imaging and intermittent orientation imaging to measure the microtexture of the evolving structure. Equilibrium structures were attained at temperatures of 250, 350, and 450ºC. Statistics of the distributions indicate that the (111) texture component strengthens due to the preferential growth of these grains. In-situ observation shows the migration of grain boundaries to their equilibrium positions and provides information on the kinetics of the process.

9:30 AM

THE CHARACTERIZATION OF TEXTURES OF THIN FILMS BY ELECTRON DIFFRACTION: DAVID E. LAUGHLIN[1]; Bin Lu[1]; Li Tang[2]; David N. Lambeth[3]; [1]Carnegie Mellon University, Department of Materials Science and Engineering, Pittsburgh, PA 15213; [2]IBM, San Jose, CA; [3]Data Storage Systems Center, Materials Science and Engineering Department

Textures which develop in thin films can be studied both qualitatively and quantitatively by means of electron diffraction. For a textured thin film, reciprocal space consists of rings of reflections, in which each ring which has the same reciprocal spacing ($1/d_{hkl}$) is located on the same spherical shell whose radius is proportional to ($1/d_{hkl}$). Accordingly, if an electron diffraction pattern (EDP) is taken with the incident beam parallel to the texture axis, a ring pattern consisting of those rings which are perpendicular to the texture axis will be present. The relative local intensity of these rings depends on their lattice spacing (d_{hkl}), multiplicity, and structure amplitude. More information about the texture can be obtained by tilting the film about an in-plane axis. In this case, additional arcs appear. The appearance of these arcs at different tilting angles depends on the degree of texture in the thin film. In this talk we will present examples of ring patterns with tables of relative ring intensities for structures with various Bravais Lattices. The details of how an EDP changes as the film is tilted away from the texture axis will be presented for some specific textured thin films. This work was sponsored in part through the Data Storage System Center at Carnegie Mellon University, by the National Science Foundation ECD 89-07068. The government has certain rights to this material. DEL also acknowledges partial support from NEDO.

9:50 AM INTERACTIVE SESSION

10:40 AM

GRAIN COMPETITION DURING THE DEPOSITION OF THIN FILMS: J. SANCHEZ[1]; [1]University of Michigan, Department of Materials Science and Engineering, Ann Arbor, MI 48109 USA

The evolution of deposited film microstructure has been the subject of many theoretical, experimental and simulation studies, and has significant importance for the continued development of technologies such as microelectronic and thin film magnetic data storage devices. However, a general understanding has not yet emerged which is inclusive of the many factors and processes controlling film microstructure and morphology development during deposition. This situation is in part due to the lack of experimental data which provide complete grain size, texture orientation and roughness/morphology characterization as a function of thickness as a film evolves during deposition. We present such a characterization of high-rate room temperature sputtered Al films, from 0.1 mm to 1.0 mm in thickness (h), for which transmission electron microscopy, x-ray pole figure analysis and atomic force microscopy provided quantitative grain size, textureand roughness results, respectively. Columnar grain size (d) of the films varied as d a $h^{0.9}$, indicating significant grain boundary migration/growth during the deposition. The Al (111) fiber texture evolved from a relatively random film (below 0.2 mm thickness) to approximately 90% Al (111) volume fraction at 1.0 mm thickness. The roughness, defined as rms height variation (H_{rms}), increased with film thickness. However when properly scaled by either grain size or thickness length scales, (H_{rms}/d) and (H_{rsm}/h) decreased with thickness, indicating significant film smoothing as the morphology and microstructure evolve during growth. These results will be discussed in terms of growth-competitive processes which may operate during film formation from the vapor. We also review of the size-, morphology- and crystallographic orientation-dependent competitive processes that may operate during the vapor deposition of metal films. Size dependent grain or domain competition may be due to the preferential incorporation of adsorbed but migrating species at the boundary between adjacent grains, where the preference for incorporation into the larger grain is due to the effects of boundary curvature at the surface, without actual boundary migration. In addition typical boundary motion/grain growth may drive the grain size evolution, driven by grain boundary curvature and energy minimization. Orientation-dependent competition may occur via processes such as preferential orientation of film "nuclei", preferential adatom incorporation into favorably oriented (low surface energy) crystal faces, preferential boundary motion to consume high surface energy grains, preferential growth of rough surfaces which provide easy sites for adatom incorporation, and favored growth of mis-oriented crystal facets.

11:00 AM

GRAIN GROWTH IN DISPERSION HARDENED COPPER FILMS: P. MÜLLNER[1]; D. Weiss[1]; J. Greiser[1]; P. Gumbsch[1]; E. Arzt[1]; [1]Max-Planck-Institut für Metallforschung, Sesstr. 92, Stuttgart D-70174

Oxide dispersion strengthened (ODS) copper films are potential materials for high temperature applications of metallic thin films. The desired microstructure of such a film consists of densely distributed particles (high strength at elevated temperature) in a matrix with large grains (minimizing diffusion along grain boundaries). We consider grain growth in 1um thick oxide dispersion strengthened (ODS) copper thin films. Two types of films were produced by magnetron sputtering of two binary copper alloys with 1 at % Y (CuY films) and 1 at % Al (CuAl films), respectively, onto silicon with a silicon nitride layer. The dispersoids were formed after deposition by internal oxidation during anneal-

ing in vacuum. Annealing experiments have been performed with films on the substrate and with free-standing films at temperatures between 400ϒC and 850ϒC for 1 h to 68 h. The dispersoids are homogeneously and densely distributed in CuAl films. In CuY films, the particle density is higher at twin boundaries than in the grain volume. The final grain size varies between 1um and 10um and depends on film type and annealing parameters. The final grain size distribution is narrow. In an intermediate stage, however, the grain size distribution of films with substrate is bimodal indicating abnormal grain growth. This study demonstrates that it is possible to form large grains with a homogeneous and dense dispersion of oxide particles in copper films on the path of internal oxidation of binary alloys. Grain growth and oxide formation are achieved in the same heat treatment.

11:20 AM
INFLUENCE OF PRECIPITATES ON GRAIN STRUCTURE EVOLUTION IN THIN FILMS: STEFAN PETER RIEGE[1]; Carl V Thompson[2]; Harold J Frost[3]; [1]MIT, Dept. of Materials Science and Engineering, Room 13-4042, 77 Massachusetts Avenue, Cambridge, MA 02139; [2]MIT, Dept. of Materials Science and Engineering, Room 13-5069, 77 Massachusetts Avenue, Cambridge, MA 02139; [3]Dartmouth College, Thayer School of Engineering, Hanover, NH

We have extended a 2D front-tracking simulation of grain growth to treat the effects of precipitates on the evolution of grain structures during annealing of thin films. In our simulation, capilarity-driven boundary motion occurs with a velocity proportional to the local curvature, and force balances are imposed at grain boundary triple junctions. When boundaries come into contact with precipitates, boundary motion is assumed to be pinned. We find that even a small volume fraction of precipitates retards grain growth, lowers the ultimate average grain size, and leads to significant changes in the grain size distribution. Comparisons will be made between the results obtained using our front-tracking code, and results obtained by others using different techniques. We will also report investigations of the interplay of precipitate effects and other phenomena which lead to grain growth stagnation in thin films, focusing on the statistical characteristics of stagnant grain structures. Comparisons between simulations and experimental observations on Al-1%Cu films will also be reported.

11:40 AM
STRESS-INDUCED DIFFUSION AND BREAKDOWN IN THIN FILM OF NANOCRYSTALLINE ZIRCONIA: ALEXANDRE ZHILYAEV[1]; Jerzy Szpunar[1]; [1]McGill University, Department of Metallurgical Engineering, 3610 University Street, Montreal, Quebec H3A 2B2 Canada

Nanocrystalline oxide scales formed on the substrate of Zr-2.5%Nb alloy have volume larger than that of the metal and compressive stress built up in the scale. This stress and its resultant effect can be of decisive importance in the oxidation behavior of zirconium alloys. There are two major stages in oxidation process: the first is when growth stress slows down oxidation kinetics, and the second stage represents an acceleration of the oxidation process which is caused by relieving the stress in film. For ZrO2 film, there are two mechanisms of stress relieving: detachment of the film at or near the oxide/metal (O/M) interface and the failure (cracks) throughout the entire oxide film. Both of these mechanisms lead to a decrease of the thickness of a non-porous, protective layer, and as a result to an acceleration of oxidation kinetics. Depending on conditions of oxidation process (stress, partial oxygen pressure, temperature, etc. three scenarios of the process are possible. First, the gas/oxide interface never reaches the metal substrate what means that the oxidation kinetics obeys the power law with lower constant rate. Second, there is an equilibrium of two processes that keeps a thin protective. The third possibility is that when cracking destroys the protective oxide scale and the metal substrate contacts with oxygen directly. In this case, the process of oxidation consists of repeating sequence - oxidation and breakdown. The present paper presents results of analytical solution of diffusion equations describing oxygen diffusion through oxide scale with two moving boundary conditions under applied stress. Transcendental equation for thickness of protective layer was calculated and plotted as function of the stress built up in the oxide and rate of moving external G/O interface. Possible applications of the results obtained for the practical use are discussed.

12:00 PM LUNCH

Steels-2

Thursday AM
June 18, 1998

Room: Rangos Hall-Room 3 (2nd floor)
Location: University Center

8:30 AM INVITED PAPER
MISORIENTATION DEPENDENCE OF GROWTH RATE IN SECONDARY RECRYSTALLIZATION IN SILICON IRON: BEVIS HUTCHINSON[1]; Hotaka Honma[1]; [1]Swedish Institute for Metals Research, Drottning Kristinas Väg 48, Stockholm S-114 Sweden

The first aim of this work was to ascertain whether the growth rate of secondaries is a function of their orientation or, more specifically, their misorientation from the exact Goss position. Experiments were carried out using commercially processed HiB sheet which was received in the final as-cold rolled gauge. This was subsequently heat treated in a laboratory furnace to obtain primary recrystallisation/decarburisation and secondary recrystallisation. A novel technique was adopted to study the relative growth rates of grain having different misorientations from Goss. Details of this method will be presented. Results show that the growth rate varies markedly with misorientation and is somewhat more sensitive to tilts around the transverse direction than around the rolling direction. By combining the experimentally determined growth rate behavior with the texture existing in the primary recrystallised condition it is possible to model the final texture on the assumption that the 'nucleation' stage is not orientation-specific. Comparison of these calculations with texture measurements made on secondary recrystallised sheet allows conclusions to be drawn regarding the relative importance of the 'nucleation' and growth stages in controlling the Goss texture evolution.

9:10 AM
AUSTENITE GRAIN GROWTH AND PRECIPITATE DISSOLUTION IN MEDIUM CARBON MICROALLOYS STEELS: GUANGJUN CAI[1]; J. D. Boyd[1]; [1]Queen's University, Department of Materials and Metallurgical Engineering, Kingston, Ontario K7L 3N6 Canada

Austenite grain coarsening and precipitate dissolution have been studied in 2 grades of medium carbon microalloyed steels: SAE 1045 + V and SAE 1045 + V, Nb. The materials were heated to temperatures ranging from 900ϒC to 1300ϒC at rates of 10ϒC/s and about 3ϒC/s, and held isothermally for periods from 10 seconds to 60 minutes respectively. Kinetic data for austenite grain growth and precipitate dissolution under these conditions were obtained. Both normal and abnormal grain growth were observed. Abnormal grain growth occurred either in the very early stage of isothermal holding or during heating at high temperatures. Under some conditions there was a transition of grain growth modes from normal to abnormal and back to normal. The occurrence of a particular grain coarsening mechanism is related to the distribution of carbonitride precipitates (Nb(C, N), V(C, N) and some Ti(C, N)) present at each stage. A model was developed to predict the variations in grain size of microalloyed forging steels during induction reheating and furnace reheating.

9:30 AM
THE EFFECT OF MAGNETIC FIELD ON GRAIN GROWTH: T. WATANABE

Abstract not available.

9:50 AM INTERACTIVE SESSION

10:40 AM

EVALUATION OF METHODS FOR ASSESSMENT OF GRAIN SIZE AND GRAIN COARSENING IN Al-TREATED STEELS: W. T. COOK[1]; P. F. Morris[1]; C. Bell[1]; [1]British Steel plc, Swinden Technology Centre, Moorgate, Rotherkam UK

The prior austenite grain size in heat treatable engineering steels is critical to their heat treatment response and subsequent properties. Testing standards contain a number of methods for assessing grain size. However, McQuaid Ehn (carburizing) is probably the most common method used for material QA assessments, carried out at a standard temperature of 925ϒC (presently the most used temperature used for carburizing). An alternative method, involving quenching to martensite, is being introduced into some material standards and both methods can be used for assessment of grain coarsening characteristics. However, the results obtained from the two methods frequently differ, McQuaid Ehn generally giving smaller values. Work has been carried out to highlight the differences in grain coarsening characteristics obtained in Al-treated steels when assessed by the two methods and to evaluate the reasons for the differences. Additionally, the grain coarsening characteristics of low (0.005%) and high (0.010%) nitrogen steels are compared and it is suggested that prior thermo-mechanical history can influence significantly the grain coarsening temperature. The difference in grain coarsening characteristics obtained test pieces may indicate potential problems with fine grain sizes in carburized components, particularly where higher carburizing contemplated.

11:00 AM

GRAIN GROWTH CHARACTERISTICS OF MICROALLOYED STEELS UNDER NON-EQUILIBRIUM THERMAL CYCLING: D. J. EGNER[1]; R. C. Cochrane[1]; [1]The University of Leeds, Department of Materials, Leeds LS2 9JT United Kingdom

Microalloyed steels are now widely accepted for use in welded fabrications, particularly for offshore applications. As such, tight control of the formation of heat affected zones (HAZ's) during welding has become necessary. In order to fully predict and hence control HAZ formation a comprehensive understanding of grain growth characteristics in these steels must be achieved. At present models exist to predict HAZ formation by combining heat flow equations, equilibrium solubility considerations of pinning particles and conditions for grain growth. Such a treatment limits the effectiveness of these models as grain growth during welding occurs under non-equilibrium conditions, particularly when considering such fabrication routes as laser welding. An understanding of grain growth specific to the conditions observed during welding need, therefore, to be adopted to advance such modeling. Presented here are austenite grain growth studies of various microalloyed steels, after both isothermal and anisothermal heating. In the latter condition, heating rates up to those encountered in welding were studied. Current theories of austenite grain growth during welding implicitly assume that there are no intrinsic differences in grain growth behavior above the precipitate solvus. Analysis of the data from this study suggests this assumption may be invalid above certain heating rates.

11:20 AM

GRAIN BOUNDARY CHARACTER DISTRIBUTION IN NICKEL OXIDE SCALES DOPED WITH CERIUM: F. CZERWINSKI[1]; J. A. Szpunar[1]; [1]McGill University, Department of Metallurgical Engineering, 3610 University Street, Montreal H3A 2B2 Canada

The grain boundaries in protective oxides act as so called "short circuit paths" for diffusion and have an essential influence on the oxidation resistance of engineering materials. It was found that a significant reduction in grain boundary diffusivity can be achieved by trace addition of elements having a high affinity to oxygen. Since the grain boundary diffusivity is related to grain boundary structure and energy, one can suspect that reactive elements altered grain boundary characteristics. In order to verify this hypothesis, the experiment was performed using nickel oxide grown on polycrystalline nickel at temperature of 800ϒC. As a reactive element, cerium in the form of ion implants and nanocrystalline coatings, was used. A reduction in the oxide growth rate was accompanied by a finer grain size and changes in the crystallographic texture. While in pure nickel oxide, a <110> fibber texture oriented along the growth direction dominates, in oxide doped with cerium the fibre texture axis was a <100>. A numerical analysis of the orientation distribution functions of grains, obtained from x-ray measurements, shows that oxide formed on pure Ni contains 3% low-angle grain boundaries, 2% twins and 14.3% of the other coincidence site lattice boundaries with sigma up to 51. The presence of reactive element did not change substantially the grain boundary character distribution. In order to explain the diffusion suppression, an analysis of grain boundary chemistry was performed using Nan-probe in electron microscope. As a result of this study, the mechanism of changing the grain-boundary diffusivity by reactive element is proposed.

11:40 AM

GRAIN GROWTH AND TEXTURE EVOLUTIONS IN NON-EQUILIBRIUM MICROCRYSTALLINE HIGH SILICON STEEL: M.V. ANISIMOVA[1]; E.I. Poliak[1]; [1]Department of Plastic Deformation of Special Alloys, Moscow State Steel & Alloys Institute, Leninski Prospekt, 4 Moscoa 117936 RUSSIA

Microcrystalline materials obtained by rapid solidification inherit considerable through thickness inhomogeneities of microstructure, texture, mechanical properties, etc. They provide large additional driving forces for microstructure transformations during processing. The evolution of microstructure and texture was studied for annealing and cold working + annealing of microcrystalline 4.8 % Si steel bands with thickness of 0.2 mm obtained by conventional two roll casting technique. In the bands, both quenched down to room temperature and coiled at 800 C before cooling, non-homogeneous through thickness grain size, texture and microhardness distributions were detected. In as-quenched bands these distributions are inverse to those observed in coils. Both types of bands undergo primary recrystallization followed by intensive normal grain growth. This is indicative of non-equilibrium states of bands and of the existence of high strain energy and its gradients resulting from rapid thermal compression and deformation in the roll gap during solidification. However, recrystallization and grain growth, as well as texture evolution in as-quenched bands exhibit the behavior inverse to that observed in coiled bands thus reflecting the differences in grain size and texture distributions prior to annealing. This inverse behavior is attributed to the inverse direction of strain energy gradients prior to annealing. Cold rolling with small (5-10%) reductions is shown to bring about additional stress gradients thus enhancing the differences in recrystallization behavior. This is in contrast with the effect of larger reductions. The general trend, described by a phenomenological model, is that the initial stages of recrystallization and grain growth are mainly controlled by strain energy gradients rather than by strain energy. The factors which enhance these gradients facilitate the onset of recrystallization and the texture transformation, and accelerate their kinetics. The initial stages proceed as to sharpen microstructure inhomogeneities, while at the latter stages the inhomogeneities are constantly reduced indicating the change in the driving force.

12:00 PM LUNCH

THURSDAY PM

Grain Boundary Properties

Thursday PM
June 18, 1998

Room: Rangos Hall-Room 1 (2nd floor)
Location: University Center

1:30 PM INVITED PAPER

EFFECTS OF GRAIN GROWTH ON GRAIN BOUNDARY CHARACTER DISTRIBUTIONS: G. PALUMBO[1]; [1]Ontario Hydro-Nanometals, Strategic Partnership in Advanced Materials, Toronto, ON M8Z 5S4 Canada

The optimization of grain boundary character distributions (usually to achieve a large population of low Σ CSL boundaries) has recently emerged as a technically-viable and cost-effective means of achieving significant performance improvements in practical engineering mate-

rials (e.g., enhanced ductility, creep resistance, fatigue resistance, weldability etc.). In this work, theoretical findings and experimental results from a broad spectrum of commercial metals and alloys (e.g., stainless steels, precipitation-hardened superalloys, lead and lead-alloys, interstitial-free steels, electrical steels etc.) are presented which show that consideration of mobility differences between low Σ and general boundaries during grain growth can be applied toward the optimization of conventional thermomechanical processes in order to achieve significant increases in the frequency of low Σ CSL grain boundaries. Texture, relative grain boundary energies, and boundary- solute interactions, are shown to be controlling factors in the evolution of the grain boundary character distribution.

2:10 PM

ABNORMAL TEXTURE DEVELOPMENT IN COLD ROLLED $Ni_{76}Al_{24}$(B) DURING RECRYSTALLIZATION: S. GHOSH CHOWDHURY[1]; R. K. Ray[1]; [1]Indian Institute of Technology, Department of Materials and Metallurgical Engineering, Kanpur 208016 India; [1]National Metallurgical Laboratory, Materials Characterization Division, Jamshedpur 83107 India

$Ni_{76}Al_{24}$(B) is cold rolled up to 85% reduction without any noticeable crack formation. Texture measurements were undertaken on the partly and fully recrystallized samples. Texture after primary recrystallization has been found to be invariably weak (max. intensity of about I SR) compared to the texture of cold rolled material (max. intensity of SR). However, some discernible features observed in the ODF after recrystallization at 850ϒC are the rotated cube component {025}<100> and the Goss component {0ll}<l00>. The rotated cube is also present after recrystallization at 950ϒC for 1 hr; whereas the Goss orientation is markedly higher than its intensities in the earlier cases. This clearly indicates that grain growth after primary recrystallization aids in the formation and growth of the Goss oriented regions. It has been found that the very weak texture produced during pre-recrystallization stage does not involve any reorientation of grains. The observed weakening is attributed to the transformation of DO_{22} structure (the structure after 85% cold rolling [1]) to $L1_2$ structure. This transformation generates lot of internal stresses which get relaxed by the formation of twins. These twins also lead to weak texture by the fragmentation of grains. Later, high nucleation rate coupled with limited growth rate lead to the starting texture before recrystallization to be retained after the process is complete. In the course of grain growth, the Goss orientation grows and becomes prominent.

2:30 PM

ANISOTROPIC BIAXIAL CREEP OF STRESS-RELIEF ANNEALED ZIRCALOY-4 CLADDING: GRAIN SHAPE AND TEXTURE EFFECTS: E. A. PREBLE[1]; B. V. Tanikella[1]; K. L. Murty[1]; Y. S. Kim[2]; Y. H. Jung[2]; [1]North Carolina State University, Raleigh, NC 27695-7909 USA; [2]Korea Atomic Energy Research Institute, Daeduk Danji, Taejon Korea

Biaxial creep behaviors of Zircaloy-4 cladding are investigated following stress relief anneals under varied ratios of hoop to axial stresses by internal pressurization superimposed with axial load. Both hoop and axial strains were monitored, and creep data were obtained at various stress ratios from which creep loci were constructed at constant energy dissipation. Zircaloy tubing following two different heat treatments were tested; one stress-relieved and the other partially recrystallized referred to as A and B respectively. Both A and B exhibit elongated grains in the r-0 plane along the axial direction. X-ray diffraction techniques were used to measure the textures which were then described quantitatively in terms of the crystallite orientation distribution functions (CODF's). These CODF's were employed to predict the anisotropy parameters R and P, and the anisotropic creep behavior. Since prism slip is known to be the operating slip system in these low c/a ratio materials, we made predictions based on the CODF-Creep model with prism slip as the dominant slip system. The current model does include the contributions from other slip systems although the major contribution is from a slip mode which is made the dominant system by appropriate choice of the reference stresses. Thus the effects of other slip modes and their combinations could be investigated. Distinct deviations were noted between the prism-slip model predictions and the experimental loci whereas the earlier results on recrystallized Zircaloy cladding gave good correlation. These differences are believed to arise from grain shape anisotropy in the stress-relieved material. The relatively small (equiaxed) grain size along the hoop and radial directions results in grain boundary sliding leading to stress enhancements along these directions, whereas such boundary sliding is not expected along the axial (rolling) direction. Incorporation of the directional dependence of such stress enhancements was earlier shown to yield good correlation between the experimental data on equi-biaxial loading of Zr and Ti alloys. Here, we extend these analyses to include other stress ratios and the entire creep locus in the first quadrant (tensile stresses) and demonstrate the applicability of consideration of grain shape anisotropy in correlating the anisotropic creep behavior of stress-relieved materials. However, for low stress-ratios ($\sigma\theta/\sigma_z \leq 0.5$) where contractile hoop strains are noted, the data seem over-corrected due probably to the fact that CBS may not strongly influence the Poisson strains required for volume conservation. Further work is underway to explore other options in this regime. This work is supported by grants from the National Science Foundation and the EPRC at NCSU.

2:50 PM INTERACTIVE SESSION

3:40 PM INVITED PAPER

GRAIN BOUNDARY MOBILITY IN METALS: THE CURRENT STATUS: G. Gottstein[1]; L. S. Shvindlerman[1]; D. A. MOLODOV[1]; [1]Institut fur Metallkunde und Physik, RWTH Aachen, Aachen D-52074 Germany

The current status of the principal aspects of grain boundary mobility in metals is considered: analysis of physically correct experimental methods, used to measure the mobility of single grain boundaries; orientation dependence of grain boundary mobility and the compensation effect in grain boundary activated processes; impurity influence on grain boundary mobility in pure metals; impurity drag theory, extended to include the interaction of adsorbed atoms; effect of grain boundary phase transitions on grain boundary mobility; steady-state motion of a grain boundary system with the triple junction and the mobility of the triple junctions; motion of the planar grain boundaries in bismuth-bicrystals driven by a magnetic field.

4:20 PM

MAGNETICALLY FORCED GRAIN BOUNDARY MOTION IN BISMUTH-BICRYSTALS: D. A. MOLODOV[1]; G. Gottstein[1]; F. Heringhaus[2]; S. Shvindlerman[3]; [1]RWTH Aachen, Institut Für Metallkunde Und Metallphysik, Aachen D-52056 Germany; [2]National High Magnetic Field Laboratory, Tallahassee, Florida 32310 USA; [3]Russian Academy of Sciences, Institute of Solid State Physics, Chernogolovka 142432 Russia

Results of investigations of grain boundary migration under a magnetic driving force in bi-crystals of high purity (99.999%) bismuth will be presented. The experiments were carried out using the 20 T Bitter magnet in the National High Magnetic Field Laboratory in Tallahassee, Florida. For the first time a defined planar grain boundary in a specially grown bicrystals was moved by means of a magnetic driving force. The mobility of 90ϒ<112> symmetrical and asymmetrical boundaries was investigated. The misorientation angle between trigonal axis in both crystals of bicrystals was chosen to be 90ϒ in order to gain the maximum possible magnetic driving force. The temperature and driving force dependence of grain boundary mobility will be discussed. By changing the position of the bicrystal with regard to the applied magnetic field the direction of the driving force could be inverted, and correspondingly boundary motion in the opposite direction was observed. The determined mobility for the 90ϒ<112> asymmetrical boundary was found to be distinctly different in opposite directions. For the chosen bicrystal crystallography the boundary moved faster, when the trigonal axis c in the growing grain was closer to the direction of motion.

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STEADY-STATE MOTION OF TRIPLE JUNCTIONS: THEORY AND EXPERIMENT: G. GOTTSTEIN[1]; U. Csubayko[1]; L. S. Shvindlerman[1]; V. G. Sursaeva[1]; [1]Institut für Metallkunde und Metallphysik, RWTH Aachen, Aachen, D-52074 Germany

It is implicitly suggested in all studies of grain boundary migration and grain growth that triple junctions do not drag grain boundary migration and their role in the process is reduced to preserving the thermodynamically equilibrium angles where grain boundaries meet. Firstly the idea that the triple junction may have the finite own mobility was put forward in 1987. In the current presentation: The main features of one of the grain boundary systems with the triple junction where the steady-state motion is possible are considered. The special technique of in-sity observation and recording of the triple junction motion and the results of the experiments on the tricrystals of Zn are reported. The kinetics are quantitatively discussed in terms of a triple junction mobility. Their impact on the kinetics of microstructure evolution during grain growth is outlined.

5:00 PM
DIRECT MEASUREMENT OF NICKEL GRAIN BOUNDARY MOBILITY USING THE IMPURITY DRAG EFFECT MODEL OF CAHN-LUCKE AND STUWE: R. LEGALL[1]; G. Liao[1]; G. Saindrenan[1]; [1]ISITEM, Labo Genie Des Materiaux, Rue C. Pauc, BP90604, Nantes, Cedes 03 F44306 France

The application of in-situ heating scanning electron microscope to the study of the recrystallization of cold worked nickel reveals the process of grain boundary migration. The velocity of grain boundary during recrystallization is plotted against the driving force for grain boundary migration deduced from initial deformation ratios. These plots have the characteristic sigmoidal form and shows an apparent low rate of grain growth at low deformation ratio. It is shown that grain boundary velocity has not a linear relationship with its driving force and could be well explained by the Cahn, Lücke and Stüwe theory of impurity drag effect. The mean values of the mobility and of the interaction energy between moving general grain boundary of nickel and sulfur are deduced from the experimental results at the temperature of 455ϒC. These study shows that it is possible to use the Cahn and Lücke and Stüwe impurity drag model to measure mobility value, but because of the assumptions of the model the value of interaction energy is not realistic.

5:20 PM ADJOURN

7:00 PM
CONFERENCE BANQUET, The LeMont

Boundary Migration

Thursday PM — Room: Rangos Hall-Room 3 (2nd floor)
June 18, 1998 — Location: University Center

1:30 PM INVITED PAPER
ANALYSIS OF SECONDARY RECRYSTALLIZATION OF GRAIN ORIENTED SILICON STEEL BY SYNCHROTRON X-RAY TOPOGRAPHY: YOSHIYUKI USHIGAMI[1]; Kenichi Murakami[1]; Takeshi Kubota[1]; [1]Steel Laboratories, Nippon Steel Corporation, 20-1 Shintomi, Futtsu, Chiba-ken 293 Japan

For the analysis of secondary recrystallization kinetics, synchrotron x-ray topography has been applied to the in situ observation of secondary recrystallization in grain oriented silicon steel. Firstly, selective growth (orientation dependence of grain growth) behavior was studied by observing the migration behavior of the following two grains; {110}<001> and {110}<115> grains. It was found that {110|<001> grain, which has higher frequency of coincidence grains in the primary recrystallized matrix, starts to grow at lower temperature and thus grows preferentially compared to {110}<115> grain. This selective growth mechanism are explained by the modified Hillert's model of grain growth, which takes the grain boundary characteristics into account. Secondly, in the grain growth process, substructures were found to form in the secondary recrystallized grains. As secondary recrystallized grains grow, crystal defects generate behind the growing interface with rearrangement of atoms. Some defects annihilate and some polygonize to form subboundaries, which successively grow along the grain growth direction and affect as a retarding force of grain growth.

2:10 PM
GRAIN BOUNDARY MIGRATION AND ROLE OF CSL BOUNDARIES SURROUNDING GOSS GRAINS DURING SECONDARY RECRYSTALLIZATION OF AN Fe3%Si ALLOY (GRADE Hi-B): A. AMIRI[1]; T. Baudin[1]; R. Penelle[1]; [1]Université de Paris Sud, Laboratoire de Métallurgie Structurale, URA 1107, Bât.410, Orsay, Cedex France

Industrial production of Fe3%Si sheets, grade Hi-B, is essentially based on the development by secondary recrystallization of a sharp Goss texture {110}<001>. The purpose of this study is to clarify the mechanisms of the Goss grain growth. Therefore we studied the grain boundary migration and analyzed the growth of several Goss grains versus temperature So an investigation on the abnormal grain growth behaviour has been performed by analyzing the Goss grain vicinity by Orientation Imaging Microscopy technique [1] which allows to reconstruct grain boundary maps from measurements of individual orientations determined by the Electron Back Scattered Diffraction. The grain boundary character distribution, around a Goss grain, was analyzed. At the primary recrystallized state, as the Goss grains have not a size larger than that of the others the abnormal grain growth is not driven by the grain size effect. It appears that, in presence of AIN and MnS precipitates, the Goss grain growth during secondary recrystallization is associated to a high mobility of CSL boundaries [2,3]. More precisely, the onset of the abnormal grain growth would be controlled by the near Σ9 CSL boundaries [4]. However, the Σ9 boundaries would not be the only factor for subsequent growth because Σ9 boundaries surrounding the Goss grains are rarely observed. Moreover Σ5 CSL boundaries seem to play an important role during the Goss grain growth.

2:30 PM
INFLUENCE OF INHERENT INHIBITION ON THE RELATIONSHIP BETWEEN GRAIN SIZE AND SECONDARY RECRYSTALLIZATION TEXTURE IN ORIENTED SILICON IRON: S. CICALÈ[1]; S. Fortunati[1]; G. Abbruzzese[1]; [1]Centro Sviluppo Materiali, V.le Brin, 218-I-015100, Terni Italy

The existence of a relationship between the average grain size, measured after primary recrystallization, and magnetic properties (texture) after secondary recrystallization of grain oriented silicon steel, produced by injected inhibitors technology, is well established. In the present paper such a relationship is investigated for different slab reheating temperatures. As a new result the investigation shows up this temperature is a relevant parameter influencing the above correlation. In fact it is here shown how the slab reheating temperature strongly affects the presence of second phase particles, which inhibits the grain growth during primary recrystallization annealing (inherent inhibition), and consequently modifies the primary recrystallization texture. Therefore the optimal primary recrystallized grain size, in order to obtain good final magnetic properties, has to be generated tuning the various process parameter according to defined slab reheating temperature.

2:50 PM INTERACTIVE SESSION

3:40 PM INVITED PAPER
EXTRACTION OF FREE ENERGIES AND MOBILITIES OF GRAIN BOUNDARIES FROM THE GEOMETRY OF MICROSTRUCTURES: A. D. ROLLETT[1]; W. W. Mullins[1]; B. L. Adams[1]; D. Kinderlehrer[1]; [1]Carnegie Mellon University, Department of Materials Science and Engineering, Pittsburgh, PA 15213 USA

Detailed descriptions of the properties of grain boundaries as a function of misorientation (and inclination) will be of great value in many systems and applications. We describe a new approach to extracting grain boundary excess free energy and (curvature driven) boundary mobility as a function of crystallographic type. The method depends on measuring very large numbers of triple junction (TJ) configurations in order to obtain statistically valid samples of relationships between energies (or mobilities) of every combination of type. The method provides relative energies (mobilities) over the entire fundamental zone and therefore requires calibration with absolute measurements of at least one reference type that is obtained independently. The extraction of boundary energies assumes local equilibrium at each TJ thus permitting the application of Herring's relations. The method is illustrated by an application to the case of a material with a strict fiber texture for which the boundary type can be simplified to a one-parameter description. The extraction of mobilities assumes that boundary velocity is proportional to energy and curvature but does not require equilibrium at each TJ. As for boundary energies, the set of relative mobilities must be calibrated by the measurement of the absolute mobility at least one boundary type. Preliminary results of serial sectioning experiments on copper and aluminum polycrystalline samples are described.

4:20 PM

SECONDARY RECRYSTALLIZATION IN BINARY STOICHIOMETRIC Ni3Al: TOSHIYUKI HIRANO[1]; Masahiko Demura[1]; Easo P. George[2]; Osamu Umezawa[1]; [1]National Research Institute for Metals, Mechanical Properties Division, 1-2-1, Sengen, Tsukuba, Ibaraki 305 Japan; [2]Oak Ridge National Laboratory, Metals and Ceramics Division, 1 Bethel Valley Road, Oak Ridge, Tennessee 37831-6093 USA

Little is known about secondary recrystallization in binary stoichiometric Ni3Al because of the difficulty in sample preparation due to grain boundary brittleness. So far, we have reported an extensive ductility in directionally solidified binary stoichiometric Ni3Al (>60% tensile elongation at room temperature). With this sample it is possible to study the secondary recrystallization with little influence of ternary elements such as boron and deviation from stoichiometry. In this paper, we present some new findings about characteristics of boundary migration, and evolution of texture and grain boundary character distribution. Large grained-structure (>10mm in diameter) was obtained by annealing at 1573K for 10 hours of cold-rolled sheet of 1mm thickness. A number of grains spanned the thickness of the sheet, forming a "bamboo" configuration. Interestingly, the texture and grain boundary character distribution were almost featureless, i.e. they remained randomly-distributed during annealing. The grain boundary grooving on the surface showed that most of the boundaries migrated discontinuously during annealing, although no boundary segregations were observed. The results are compared to the behavior of common metals.

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STRUCTURAL CHANGES DURING GRAIN BOUNDARIES MIGRATION OF SUBMICROMETER - GRAINED ALLOY Al-3%Mg: N. K. Tsenev[1]; A. M. SHAMMAZOV[1]; [1]Ufa State Petroleum Technical University, Ufa, Kosmonavtov str. 1 450062 Russia

The present work deals with experimental studies of structural changes and kinematics of grain growth of submicrometer-grained (d < 1 mm) model alloy Al-3% Mg during annealing. The submicrometer-grained structure was obtained on Bridgmen anvils under a pressure of 6 GPa and the true logarithmic strain degree e=5. The TEM analysis of the submicrometer-grained alloy Al-3% Mg showed that in the initial state a mean grain size constituted 0.25 mm and grains were misorientated by high angles. The existence of extinction contours inside a grain body and the "blurring" of a banded contrast on grain boundaries testify to the presence of strong elastic fields. The microdiffraction pattern from an area of 0.75 mm2 has a large amount of reflexes arranged in a circle. Part of reflexes are a bit blurred, this confirms the existence of strong elastic fields. TEM methods did not reveal the presence of lattice dislocations inside a grain body. Annealing of samples in the temperature interval 373-523 K leads to considerable changes in structure of grain boundaries. Annealing at the temperature 373 K for 1 hour results in the appearance of a distinct banded contrast on grain boundaries. Grain size remains the same. These results show that at the given temperature recovery processes occur only on grain boundaries. Lattice dislocations are not revealed inside the grain body. Further increase in the temperature of annealing leads to grain growth. One should note that with increasing the grain size to 0.4-0.5 mm no dislocations are observed inside the grain body. However, as the grain size reaches 0.5-0.7 mm an aggregate of dislocations appears inside the grain body. These results show that grain boundary migration of the submicrometer - grained alloy is accompanied by concurrent precipitation of lattice dislocations. When the grain size is within the range 0.4-0.5 mm the appearance of lattice dislocations inside the grain body leads to their absorption and dissociation due to the "Mirror reflexion" law. When the grain size is more than 0.5 mm and the "Mirror reflexion" law does not act, an increase of lattice dislocation density inside the grain body occurs during annealing. On the basis of the experimental results of investigation of grain boundary migration a model of grain growth during annealing is suggested.

5:00 PM

RESEARCHING THE PERSPECTIVES OF PRODUCING POWDER NANO MATERIALS FROM ZIRKONIUM CONTAINING MINERAL RAW MATERIALS: S. V. NIKOLENKO[1]; R. M. Budkina[1]; T. B. Ershova[1]; A. M. Sundukov[1]; N. M. Vlasova[1]; L. F. Gorelova[1]; [1]Far Eastern Branch of Russian Academy of Sciences, Institute of Material Science, Khabarovsk Russia

Creation of ceramic nanomaterials with predetermined properties is one of the main tasks of contemporary material science. Among the known methods of producing powders, that combine high rate of homogeneousness and monodispersion of particles - chemical synthesis is the most perspective one. We have produced an amorphous powder containing 49% of ZrO_2 and 47% of SiO_2 (plus secondary products) from zirkonium concentrate by SolGel technology. Having been dried on air at the temperature of 100ϒC the product represents a thin dispersion powder composed from agglomerates with sizes up to 50 nm and 52% of ZrO_2. Zirconium and silicon borates, produced by the sintering of zirconium concentrate with a blend of borax and soda in respective proportion, were used as original reagents for the synthesis of the gel. The structural changes of the gel occurring in the temperature interval of 100-800ϒC were studied. We have found that at around 700ϒC ZrO_2 monowedge and ZrO_2 cubic crystal phases are formed from the amorphous powder.

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CONFERENCE BANQUET, The LeMont

FRIDAY AM

Boundary Structure

Friday AM
June 19, 1998

Room: Rangos Hall-Room 1 (2nd floor)
Location: University Center

8:30 AM INVITED PAPER

MOLECULAR-DYNAMICS SIMULATION OF GRAIN-BOUNDARY MIGRATION: D. WOLF[1]; [1]Argonne National Laboratory, Materials Science Division, Argonne, IL 60439 USA

A molecular-dynamics method for the simulation of the intrinsic migration behavior of individual, flat grain boundaries is introduced and validated. A constant driving force for grain-boundary migration is generated by imposing an anisotropic elastic strain on a bicrystal such that the elastic-energy densities in its two halves are different. For the model case of a large-planar-unit-cell, high-angle (001) twist boundary in Cu we show that an elastic strain of ~1% - 4% is sufficient to drive the continuous, viscous movement of the boundary at temperatures

well below the melting point. The driving forces thus generated (at the high end of the experimentally accessible range) enable a quantitative evaluation of the migration process during the time frame of 10^{09}s typically accessible by molecular-dynamics simulation. For this model high-angle grain boundary we demonstrate that[1] (a) the drift velocity is, indeed, proportional to the applied driving force thus enabling us to determine the boundary mobility, (b) the activation energy for grain-boundary migration is distinctly lower than that for grain-boundary self-diffusion or even self-diffusion in the melt and (c) in agreement with earlier simulations the migration mechanism involves the collective reshuffling during local disordering ("melting") of small groups of atoms and subsequent resolidification onto the other crystal.

9:10 AM
GEOMETRY OF COINCIDENT-SITE LATTICE BOUNDARIES: KAZUHIRO FUCHIZAKI[1]; [1]Kyushu University 33, Department of Physics, 99, Fukuoka 812 Japan

Recently large-scale computations, including the first principles calculations, regarding the interfacial energy between the two crystallines, which capture detailed nature of materials concerned have been made. It has been believed that the details of the bending at an interface are crucial in understanding the dependence of the interfacial energy on geometrical location of the interface. Nevertheless the similarity of the overall features of the curves of energy against misorientation for several materials suggests a common underlying physics which should not depend strongly on the material chosen. The present investigation is therefore to discuss the commonly observed characteristics in the energy curves from purely geometrical point of view. To this end I first clarify the hierarchy among the coincident-site lattice structures by adopting the continued-fraction expansion algorithm for a transformation operator between the two lattice structures. Interfacial energies are then calculated against misorientation based on a two-dimensional version of the model put forth by du Plessis and van der Merwe, which turn out to reveal a fractal energy surface with cusps at every sigma value. It is emphasized that these singularities are not attributable to structural relaxations.

9:30 AM
A MODEL FOR INCOHERENCE AT GRAIN BOUNDARIES: DARREN E. MASON[1]; [1]Department of Mathematical Sciences, Marnegie Mellon University, Pittsburgh, PA 15213-3890 USA

A fundamental question in material science is determining what role material defects play in the behavior of grain boundaries. Understanding this connection relies on resolving the behavior of the material on many scales. We propose an energetic model to describe the small scale defect structure of incoherent interfaces in an elastic polycrystal. This energy is composed of two parts: a bulk energy, density W that describes the macroscopic behavior of the material away from the interface and a nonconvex interfacial energy density σ that depends both on the microscopic lattice mismatch at the grain boundary and the relative crystallographic normal n. This mismatch is modeled using a referential coherence tensor H that measures the relative misfit at the grain boundary and serves to couple the bulk elastic deformation of the grains to small scale defect structures at the grain boundary. We study the question of minimizing this energy for a variety of boundary conditions, employing contemporary methods of multi-scale analysis and simulation. This yields predictions for the distribution and orientation of defect microstructures at the interface. In addition, we describe implications of this model on the possibility of mesoscale faceting of grain boundaries. This is joint work with David kinderlehrer.

9:50 AM
ATOMISTIC SIMULATION OF GRAIN-BOUNDARY MIGRATION OF TILT-GRAIN BOUNDARIES: BERND SCHÖNFELDER[1]; Günter Gottstein[1]; Lasar S. Shvindlerman[2]; [1]RWTH Aachen, Institut für Metallkunde und Metallphysik, Kopernikusstrasse 14, Aachen, NRW 52056 Germany; [2]Russian Academy of Science, Institute of Solid State Physics, Chernogolovka Russia

Molecular-dynamics simulations are used to investigate continuous migration of tilt-grain boundaries. It is shown that the application of an appropriate external strain to a bicrystal of Cu results in a continuous migration of flat tilt-grain boundaries. The propagation of tilt boundaries on low index planes is determined as a function of both the external driving force and the temperature. The grain-boundary velocity depends linearly on the elastic driving force, thus the grain-boundary mobility can be determined. Its temperature dependence and details of the atomic-level migration mechanism of these grain-boundaries are also investigated. It is shown that for some tilt-grain boundaries sliding and migration are coupled.

10:10 AM BREAK

10:30 AM INVITED PAPER
ROLE OF COINCIDENCE GRAIN BOUNDARIES IN SECONDARY RECRYSTALLIZATION OF GRAIN ORIENTED SILICON STEEL: Woo Jong Soo[1]; Han Chan-Hee[1]; Hong Byung-Deug[2]; JIROU HARASE[2]; [1]Pohang Iron & Steel Corporation, Technical Research Laboratories, Pohang Korea; [2]Pohang University of Science & Technology, Pohang Korea

Grain oriented silicon steels are now mainly produced by their different methods. All these methods require high temperature slab reheating technology to secure fine precipitates as inhibitors . The requirement of high slab reheating temperature causes various troubles in the production of grain oriented silicon steel and a development of the low slab reheating technology has been one of the largest target in the research and development in this field. Quite recently new technology has been announced which makes it possible to produce grain oriented silicon steel by low slab reheating temperature as 1150℃. There are many similarities in the conventional technology and this new technology. Role of coincidence boundaries in the secondary recrystallizaticn in these methods are investigated and the possibility of the future progress of technology are discussed.

11:10 AM
GRAIN GROWTH IN TITANIUM-ALUMINIDE-BASED ALLOYS WITH NANOCRYSTALLINE, MICROCRYSTALLINE AND BIMODAL STRUCTURES: O. N. Senkov[1]; F. H. (SAM) FROES[1]; N. Srsukhumbovornchai[1]; M. L. Övercoglu[2]; [1]University of Idaho, Institute for Materials and Advanced Processes, Moscow, ID 83844-3026; [2]Istanbul Technical University, Maslak, Istanbul 80626 Turkey

Results are presented on grain growth studies of the gamma titanium aluminide Ti-47Al-3Cr and Ti-48Al-2Nb-2Cr (at. %) alloys with nanocrystalline (initial grain size D_o < 100 nm), microcrystalline (D_o ~ 1 mm) and bimodal (mixture of the nano-and micro-grains) structures. The alloys were produced by a hot isostatic pressing from gas-atomized and mechanically alloyed powders and from 1:1 mixture of these powders. The grain size distribution and mean grain size were determined after annealing at temperatures in the range of 725℃ to 1200℃ for annealing times of up to 800 hours using TEM. In the case of nano-and micro-crystalline materials, grain size distributions normalized to the mean grain size were single-modal and time-and temperature- invariant. In both cases the grain growth was described by a single thermally activated rate process limited by a permanent pinning force. Grain growth in the material with bimodal structure occurred independently in the two regions of nano-sized grains and micro-sized grains, and in the same fashion as in the separately processed materials. Possible reasons for this behavior will be discussed.

11:30 AM
INTERFACIAL PHASE STABILITY IN NiNb SUPER ALLOYS: RAHUL D. BASU[1]; [1]GTRE, PB 9302, CV Raman Nagar, Bangalore 560093

A model for progressive freezing in a porous matrix with coupled heat and mass transfer is setup. A stability criterion for the moving phase boundary evolves and can be related to an earlier physical metallurgical model studied at NASA (CR 134678). The present model with a moving boundary yields a refined planar stability criterion taking

effects of porosity and thermal gradient in both liquid and solid phases. "Freckling" in Nh containing Ni super alloys is tackled as part of the project. Freckles consist mainly of NiNb (AB2 type) phases related to Laves and intermetallic phases. Some carbide is also associated with freckling. Parameters such as intent heat, diffusivity, porosity, are varied to describe effects on radial freezing. Thus the kinetic properties of the interface relate to the thermal and thermodynamic parameters of the model. Physically, the model describes a VAR. formed ingot with a disk of liquid under a line source at the origin (z axis). Vertical buoyant and convective c/Tects are neglected. Earlier work has emphasized the role of convection, whereas the present model is diffusion driven under thermal and concentration gradients.

12:00 PM CLOSING REMARKS (McConomy Auditorium)

Kinetics

Friday AM
June 19, 1998

Room: Rangos Hall-Room 3 (2nd floor)
Location: University Center

8:30 AM INVITED PAPER

THE DYNAMICS OF GRAIN GROWTH IN SLIGHTLY IMPURE MATERIALS: R. A. VANDERMEER[1]; [1]2121 Jamieson Avenue #2111, Alexandria, VA 22314 USA

Polycrystalline metals, alloys and ceramics that are subjected to sufficiently high annealing or service temperatures can undergo grain growth presumeably by curvature-driven migration of grain boundaries to reduce the grain boundary area per unit volume. In this paper isothermal grain growth kinetics (average grain size versus time) in slightly impure metals under non-steady state conditions are considered theoretically. It is hypothesized that unsaturated, migrating grain boundaries acting as impurity traps may be able to sweep up soluble impurities during grain growth, provided, of course, that there exists an ample binding energy of the impurities to the boundaries. In this analysis moving grain boundaries are treated from an irreversible thermodynamic viewpoint. An additional force acting on grain boundaries as they sweep up impurities is shown to arise from the thermodynamic reduction in grain boundary energy associated with solute segregation to the boundaries. A previously developed, volume-averaged kinetic model formulated on microstructural path considerations is further modified to include the various solute atom effects. It is shown that when the migrating grain boundaries are sweeping up impurity atoms during grain growth, additional forces act on the boundaries giving rise to a pinning-like force that can slow grain growth kinetics causing deviations from the expected ideal parabolic time dependence. The importance of the proposed solute atom sweeping phenomenon is assessed for slightly impure aluminum using earlier experimental resistivity and grain size data that seem to demonstrate the existence of a grain boundary sweeping phenomenon.

9:10 AM

STUDY OF THE SIZE DISTRIBUTION OF PRECIPITATES AND ITS EFFECT ON THE GRAIN GROWTH BEHAVIOR OF Ti-BEARING STEELS: S. W. LEE[1]; C. I. Garcia[2]; A. J. DeArdo[2]; W. Y. Choo[1]; [1]POSCO, Technical Research Laboratories, Pohang 790-785 Korea; [2]University of Pittsburgh, Dept. of MSE, 848 Benedum Hall, Pittsburgh, PA 15261 USA

The size distribution of precipitates and its effect on the gram growth behavior of Ti-bearing steels were investigated in the continuously cast Ti and Ti-Nb steels. In as-cast condition, the AC slabs which had been air-cooled after slab-cutting, contained more and finer precipitates than the WC slabs which were water-cooled after slab cutting. Also, Ti steel slab comprised the precipitates of cuboidal shape, while almost all the precipitates in Ti-Nb steel slab had the dendritic star-like morphology. The star-like precipitates easily dissolved and then changed to the cuboidal particles during reheating above 1100ϒC. At reheating stage the WC slabs had so large a tendency to the abnormal grain growth that they showed larger average grain sizes than the AC slabs. The variation in the degree of segregation with post solidification cooling rate was considered to be an important factor which derived a large difference in grain growth behaviors of the WC and the AC slabs. In the AC slabs the solute diffusion from interdendrite pool to dendrite arm could occur during slow cooling after slab-cutting. Therefore, precipitation could take place even in dendrite arm region, so that the abnormal grain growth was suppressed due to large pinning force. Meanwhile, the formation of precipitates in the WC slab would be so localized in the interdendrite pool that the abnormal grain growth was accelerated due to an insufficient grain boundary pinning force by few precipitates in dendrite arm region.

9:30 AM

AUSTENITE GRAIN GROWTH IN MICROALLOYED LOW CARBON STEELS: M. MILITZER[1]; E. B. Hawbolt[1]; [1]The University of British Columbia, The Centre for Metallurgical Process Engineering, Vancouver, BC V6T 1Z4 Canada

The kinetics of austenite grain growth has been measured in a variety of low and ultra-low carbon steels microalloyed with Nb and/or Ti. The heat treatment of the samples has been performed either employing a Gleeble 1500 thermomechanical simulator or in an air furnace. The latter was required for the ultra low carbon steels where the austenite microstructure could only be revealed by a glass etch technique which is applied at temperature. In general, it has been observed that for reheating temperatures below approximately 1100ϒC no or insignificant grain growth takes place. At a critical temperature which depends on the steel chemistry, but is in the range of 1100 - 1150ϒC, marked grain growth starts to take place. Frequently, a period of abnormal grain growth is characteristic for this stage followed by normal grain growth of the coarse grains. This behavior is indicative for dissolution of precipitates and consistent with the solubility of Nb(CN), NbC and TiC, respectively. In Ti microalloyed grades a limiting grain size is usually reached due to the presence of TiN which is stable up to the melting temperature. The pinning forces and their change with temperature have been evaluated with the statistical grain growth model of Abbruzzese and Lücke.

9:50 AM

NEW PROCESS AND TECHNOLOGY - VEAT - IN DIRECTIONAL SOLIDIFICATION OF EUTECTICS: PAUL CHRISTIAN OLARU[1]; [1]Omlet , Senior Metallurgical Aircraft Engineer, Bucharest Romania

VEAT process consists of the simultaneous application of a stationary magnetic field $B_o$of and of a variable magnetic field b(t) in the vicinity of the molten metal during the course of solidification. It shows that the grain refinement can be effective when an alloy is electromagnetically vibrated under favorable conditions concerning primarily the amplitude of the oscillating pressure. Results from experiments with eutectic Al-Al_3Ni and Al-Al_3Fe alloys are shown to demonstrate the facility is working and the accuracy of the optical temperature measurements can be evaluated. Also, results revealed that the size and shape of the crystals can be controlled both by the application either of various magnetic fields or of a com bination of magnetic fields of sufficient strength and by an adequate heat extraction rate.

10:10 AM BREAK

10:30 AM INVITED PAPER

VARIANT SELECTION DURING PRIMARY RECRYSTALLIZATION: J. J. JONAS[1]; [1]McGill University, Dept. of Metallurgical Engineering, Montreal, Quebec H3A 2B2 Canada

It has frequently been reported that highly mobile grain boundaries are associated with rotations of 30ϒ - 40ϒ about <111> in fcc metals and with rotations of 25ϒ - 35ϒ about <011> in bcc metals. However, four equivalent <111> axes are present in the former case and six equivalent <011> ones in the latter. Analysis of experimental data obtained on cold worked cubic metals undergoing recrystallization shows that the observed rotations are not equally distributed about the four fcc and six

bcc rotation axes. Instead, there is marked variant selection in favour of one (and sometimes two) of these axes. The possible causes of such variant selection are examined in turn and discussed critically.

11:10 AM

GRAIN GROWTH KINETICS IN NANOCRYSTALLINE IRON PREPARED BY BALL MILLING: A. MICHELS[1]; C. E. Krill[1]; R. Birringer[1]; [1]Universität des Saarlandes, FB 10 Physik, Gebäude 43, Postfach 151150, Saarbrücken D-66041 Germany

The small average grain size (< 30 nm) in nanocrystalline materials renders them potentially useful for the study of grain-size evolution- and the accuracy of grain growth models-over more orders of magnitude than are accessible in conventional polycrystalline materials. We have prepared nanocrystalline Fe under highly pure conditions by ball milling and investigated the kinetics of grain growth at temperatures between 300ϒC and 600ϒC. Grain-size determination was performed by x-ray diffraction peak-profile analysis. Three different grain growth models were fit to the size evolution curves a generalized "Hillert" growth law with variable exponent (used to describe normal grain growth in the absence of impurities), the Burke equation assuming a constant retarding force on moving grain boundaries (solute drag), and a third model in which the retarding force scales with grain size owing, to impurity enrichment in the grain boundaries. Based on the generalized "Hillert" analysis, a previous investigation of grain growth in ball-milled nanocrystalline Fe yielded a temperature-dependent growth exponent that reached the expected value of 0.5 only at high temperatures. In contrast, we find that the grain growth kinetics in our ball-milled Fe samples are better described by either of the two models accounting for the influence of impurities on the growth rate, despite the fact that special precautions were taken to maintain a low overall impurity level. Since both models reduce to the ideal "Hillert" model for negligible impurity concentrations, their underlying growth exponent is 0.5. This suggests that the temperature dependence of the exponent reported for ball-milled Fe is an artifact of the model used to interpret the grain growth data rather than a true description of the underlying growth kinetics.

12:00 PM CLOSING REMARKS (McConomy Auditorium)

POSTERS

(1) A TWO-DIMENSIONAL VERTEX SIMULATION GRAIN GROWTH STARTING FROM EXPERIMENTAL DATA: A. AMIRI[1]; T. Baudin[1]; R. Penelle[1]; [1]Université de Paris Sud, Laboratoire de Métallurgie Structurale, URA 1107, Bât. 410, Orsay, Cedex 91405 France

Normal and abnormal grain growth can be simulated in different ways, i.e. by Monte-Carlo,Vertex techniques, for example. The classical Monte-Carlo technique does not allow to simulate real time and space scales unlikethe vertex method. So the Vertex method has been implemented to simulate normal and abnormal grain growth, in Fe3%Si alloy, by following the displacement of vertices (triple junctions) of experimental microstructure. The experimental microstructure can be precisely introduce for the simulation [1] experimental measurements of the initial microstructure are transformed into sets of data to define the initial grain parameters for simulation. These experimental data are characterized by Orientation Imaging Microscopy [2] which allows to construct the microstructure from orientation measurements by Electron Back Scattered Diffraction. The vertices of the experimental microstructure that are the input data of the simulation can easily be located. The curvature of the boundaries adjacent to each vertex are located by the position of the neighboring vertices and the "virtual" vertices which are on this experimental curvature. The motion of each vertex is then calculated as a vector sum of the curvature-driven motions of the adjacent boundaries by the relationship : $v = 2m.\gamma\beta$ where v is the velocity, m the mobility, γ the energy and β the curvature radius of grain boundary. In a first step the Vertex method was applied to the normal grain growth in order to validate thismethod and in a second step to the secondary recrystallization in order to compare experimental [3]and simulated results.

(2) GRAIN GROWTH IN IRON (III) OXIDE POWDER UNDER ULTRASONIC TREATMENT: A.Y. Baranchickov[1]; A.N. Baronov[1]; O.N. Nickolayevich[2]; K.Vitally M.[1]; [1]Inst. for General & Inorganic Chemistry RAC, Chemical Cynergy Lab, Moscow 117905 Russia; [2]MSU, Dept. of Chemistry, Inorganic Chemistry Division, Moscow 119899 Russia

It was previously shown that ultrasonic treatment considerably affects solid state processes, changes of grain morphology and grain growth. As for ceramic materials, such information is quite insufficient. In our work we studied processes of grain growth, microstructure evolution, and sintering of iron (III) oxide powder under different intensity and duration of ultrasonic treatment. Iron (III) oxide powder obtained from nitrate was treated by ultrasound of various intensities (amplitudes of vibration were 10 - 13 mm) and duration (up to 4 hours) at the temperatures 850-950 C. Microstructure of powders was studied by XRD and SEM. SEM examination showed that grain size of treated samples was in 1.5 times larger than in control series. According to XRD data, the crystallite size growth with increase of treatment duration was observed. This fact can be explained in terms of viscous flow in annealed sample, that improves intercrystallite contacts. The increase of ultrasonic power led to crystallite size decrease due to defect accumulation in crystal structure up to new boundary formation, eventually resulting in growth of effective diffusion coefficients in ultrasonic field. Changes in microstructure influenced on the reactivity of iron (III) oxide in solid state reactions.

(3) EFFECT OF REINFORCEMENT PARTICLES ON RECRYSTALLIZATION AND GRAIN GROWTH OF SIC_p/Al COMPOSITE: YANG CAO[1]; Goujun Li[2]; Jiaxin Yao[2]; Naiqin Zhao[2]; J. A. Szpunar[1]; [1]McGill University, Department of Mining and Metallurgical Engineering, Quebec H3A 2B2 Canada; [2]Tianjin University, School of Materials Science and Engineering, Tianjin P.R. China

In this paper, a relationship between reinforcernent particles and grain growth has been carefully investigated for SiC particles reinforced aluminum metal matrix composites made by a rapidly solidified powder hot-pressing consolidation process. During hot pressing and extrusion, the recovery and recrystallization of composites are influenced by SiC particles because the extrusion pressure of composites is higher than that of the matrix alloy and hard SiC particles in the composite promote an increase in the build-up of internal stresses. The grain growth of composites during an isothermal treatment has been studied using microstructural optical analysis and microhardness measurements. The reinforcement particle distribution and particle size play an important role in the grain refinement which is attributed to heterogeneous nucleation that is linked to a small (7%) lattice mismatch between SiC and aluminum with an relationship of $(111)_{sic}(111)_{Al}$ and SiC(1μm) pining effects. At the same time, oxide debris of often alloy powders surface crushed by extrusion has also a certain role in the inhibition of grain growth. Based on the experiments performed and theoretical analysis a model has been proposed to explain this phenomenon.

(4) MICROSTRUCTURES AND GROWING MODEL OF Al_2O_3/Cu COMPOSITE COATING: YULIN WANG[1]; Naiqin Zhao[1]; Yang Cao[2]; Zianghong Dong[1]; Guojun Li[1]; [1]Tianjin University, School of Materials Science and Engineering, Tianjin 300072 P.R. China; [2]McGill University, Department of Metallurgical Engineering, Montreal, PQ Canada

Microstructures of Al_2O_3Cu composite coating by electrolytic codeposition were studied by TEM and SEM microscopy. The results show that microstructures of the coating was influenced by the place of electrode-plates, current density and plating time. The growing model of electrocrystallization in composite coating was proposed. The composite coating crystallized and grew by means of plane and spiral form.

Plane growing form plays a key role in crystallization and growth. The surface of coating appeared small mound shape at the beginning of plating, then developed a ridge shape.

(5) ON THE MICROSTRUCTURE CONDITIONS REGULATING THE INCUBATION AND KINETICS OF SELECTIVE SECONDARY RECRYSTALLIZATION IN SILICON-IRON: S. FORTUNATI[1]; S. Cicalè[1]; G. Abbruzzese[1]; [1]Centro Sviluppo Materiali, Viale B. Brin 218, I-05100, Terni Italy

The selective grain growth and secondary recrystallization (SR) of the Goss grains in grain oriented electrical steels take place during the final treatment in box annealing furnaces. The temperature at which the SR takes place influences the selectivity of the process. The whole of the phenomena which develop before the SR onset is defined as the incubation of the process, and it occurs in several hours during a very slow heating of the coils. It includes the achievement of equilibrium between the grain growth driving force and the grain boundaries restraining force (GB inhibition) as well as the selective growth of few Goss grains up to the critical size of the secondary recrystallization nuclei. In the present paper the authors discuss the influence of the main microstructure parameters on the incubation time and kinetics of the secondary recrystallization, in the case of the different production strategies for these materials. Based on theoretical considerations, computer simulations and experimental results, the main absolute parameters controlling the SR incubation time are recognized and their relative effects are quantitatively discussed. Further experiments are presented in order to show how, choosing the adequate conditions, it is possible to reduce the SR incubation time down to few minutes and still obtain a final microstructure with a sharp Goss texture.

(6) GRAIN GROWTH BEHAVIOUR OF NANOCRYSTALLINE NICKEL-IRON ALLOYS: F. CZERWINSKI[1]; H. Li[1]; J. A. Szpunar[1]; [1]Queen's University, Department of Materials and Metallurgical Engineering, Kingston K7L 3N6 Canada

Thermal stability of electrodeposited nanocrystalline Ni-20%Fe and Ni-45%Fe alloys was studied by x-ray diffraction techniques and atomic force microscopy Alloys composed initially of γ(f.c.c.) phase were annealed at 573 and 673 K for time periods up to 20 h in an inert atmosphere of argon. The evolutions of grain size, microhardness and crystallographic texture were analyzed as afunction of annealing parameters. The initial grains, approximately 5 run in size, increased after annealing up to 10-20 nm, however, the growth kinetics and the final grain size depended on the temperature. A correlation was found between the grain size and alloy microhardness which supports the validity of Hall-Petch strengthening. The phase composition was unstable and durin gannealing the α(b.c.c.) phase was detected to precipitate from the matrix of Ni-45%Fe alloy. The texture of γ phase, consisted of two fibre components of <111> and <100>, and changed during annealing. In general, the <111> component became stronger at the expense of <100>, however, the detailed changes depended on temperature and alloy composition.

(7) ON THE ROLE OF ORIENTATION CORRELATIONS IN THE GRAIN BOUNDARY CHARACTER DISTRIBUTION IN TEXTURED POLYCRYSTALS: V. Y. GERTSMAN[1]; A. P. Zhilyaev[1]; J. A. Szpunar[1]; [1]McGill University, Dept. of Metallurgical Engineering, 3610 University Street, Monteral, PQ, H3A 2B2, Canada

Among various distribution functions describing microstructure of polycrystals, two relate to the crystallite orientations, namely, crystallographic texture and misorientation distribution. In recent years, relationships between grain boundary misorientation distributions and texture have been studied both experimentally and by means of computer simulation. While there have been attempts to derive misorientation distributions from texture data only, our studies have shown that in general the relationship between the two distributions is not straightforward but rather ambiguous. Complications arise due to the orientation correlations which may exist between various crystallites of the polycrystalline aggregate. By orientation correlation we mean a tendency for grains with a certain relative orientation (i.e. misorientation) to be adjacent. These two factors, texture and orientation correlations, determine the grain boundary character distribution in a sample. Contributions of these factors to the misorientation distribution as a whole and to the fractions of specific grain boundary types are yet to be fully understood. In some materials, for example aluminum and b.c.c. alloys, grain boundary distribution is primarily determined by texture. However, the orientation correlations play a dominant role in f.c.c. alloys prone to annealing twinning. The same may be true for other materials with a high propensity to formation of special (twin) boundaries. Experimental and computer simulation results obtained on nanocrystalline monoclinic zirconia film give evidences in favor of this conclusion.

(8) MEASURING GROWTH KINETICS OF INDIVIDUAL GRAINS DURING SECONDARY RECRYSTALLISATION USING AN IN-SITU NEUTRON DIFFRACTION TECHNIQUE: ANDREW GODFREY[1]; Mark Miodownik[2]; Dorte Juul Jensen[3]; John W. Martin[2]; [1]Sandia National Laboratories, Materials Reliability Department, P.O. Box 969 MS 9403, Livermore, CA CA 94551-0969 USA; [2]University of Oxford, Department of Materials, Parks Road, Oxford OX1 3PH U.K.; [3]Risoe National Laboratory, Materials Department, Roskilde DK-4000 Denmark

An in-situ neutron diffraction method has been developed enabling the growth kinetics of individual grains to be monitored during the secondary recrystallisation of extruded MA754. This nickel based oxide dispersion strengthened (ODS) superalloy undergoes secondary recrystallisation transforming a weakly textured sub-micron grain size structure into a coarse grained structure with a strong <100> fibre texture. Using a linear position-sensitive detector, together with an Euler cradle, the diffracted intensity from an individual grain can be isolated from all other diffracted intensities and continuously monitored with time. By control of the specimen temperature the growth kinetics of individual grains can thus be investigated. The technique also provides an experimental tool for directly investigating the phenomenon of solute break away. This has been suggested as providing an explanation for the triggering of secondary recrystallisation in a number of ODS alloys. The technique is potentially applicable to any system undergoing secondary recrystallisation to produce a coarse grained structure. **This work was supported by the Commission of the European Community through the Large Installation Plan, and by the U.S. Department of Energy.

(9) ON THE STRUCTURE, PROPERTIES AND MIGRATION OF GRAIN BOUNDARIES IN PRIMARY RECRYSTALLIZED METALS: V. V. GUBERNATOROV[1]; [1]Ural Branch of RAS, Institute of Metal Physics, Yekaterinburg Russia

A new approach is proposed with respect to the structure and properties of inter crystallite (grain) boundaries (GB's) in metals subject to the primary recrystallization (PR) and also the GB movement during the collective (CR) and secondary (SR) recrystallizations. This approach is based on the concept of the GB origin. In a primary recrystallized metal almost all GB's appear as a result of collisions between the grains, which develop in the deformed and polygonized matrix. During the PR a growing grain is bounded (growth faces) by the planes possessing a maximum surface energy and, correspondingly, a maximum growth rate. When the grains stop growing, they should be bounded by the planes having a minimum surface energy. The replacement of the growth faces by the equilibrium faces determines the structure of the GB's and the grain junctions. The proposed approach to the formation of the GB's allows estimating their mobility, which is the most significant property of the GB's. It also permits determining the contribution of grain junctions to the recrystallization processes: three-, four-fold, etc. grain junctions count very much in the CP and the SR.

(10) THE FORMATION OF THE SUBSTRUCTURE DURING RECRYSTALLIZATION PROCESSES: V. V. GUBERNATOROV[1]; [1]Ural Branch of RAS, Institute of Metal Physics, Yekaterinburg Russia

It was found that under certain conditions a migrating grain boundary leaves behind it such a crystalline structure defect as a "defect bundle". One of the mechanisms responsible for the appearance of this

defect is as follows: A developing grain by-passes an area, where the growth rate of this grain is much lower than in the bulk of the material. Having by-passed this area, the grain parts cannot mate properly, because a certain misorientation builds up during their separate growth. This leads to the formation of a "defect bundle", which is subsequently reproduced by the grain boundary as it moves. The misorientation of the separately growing parts of the grain increases only when these parts absorb matrices, which differ in their texture and structure states.

(11) GRAIN GROWTH ASPECT IN THE SYSTEM WITH ANISOTROPIC GRAIN BOUNDARY ENERGY AND MOBILITY: NONG M. HWANG[1]; Chan H. Han[1]; [1]Korea Research Institute of Standards and Science, Microstructure Science Group, P.O. Box 102, Yusung-gu, Daedok Science Town, Taejon 306-600 Republic of Korea

Effects of anisotropic grain boundary energy and mobility on grain growth are studied by Monte Carlo (MC) computer simulation. Simulation shows that in the presence of the anisotropic grain boundary energy, the low energy grain boundary tends to replace the high energy grain boundary and finally, the fraction of those grains making low energy grain boundary increases with grain growth. This effect was negligible when the initial fraction of the grains making low energy grain boundaries is small. However, the effect is significant when the initial portion is large. In the case of the anisotropic grain boundary mobility, the grain boundary with low mobility tends to survive over that with high mobility. When both effects of energy and mobility are considered simultaneously, the fraction of the grain boundary with low energy and low mobility increased markedly during grain growth. The grain boundary with low energy and high mobility tends to disappear. The simulation results qualitatively agree with the previous experimental observations. The condition of low energy and low mobility is satisfied by the Σl grain boundary. Increase in the fraction of the Σl grain boundary with similar orientations will have tendency of the texture.

(12) GRAIN GROWTH IN $YBa_2Cu_3O_{7-x}$ SUPERCONDUCTIVE CERAMICS: M. F. IMAYEV[1]; D. B. Kazakova[1]; [1]Russian Academy of Sciences, Institute for Metals Superplasticity Problems, Khalturina 39 UFA 450001 Russia

Grain growth at annealing of $YBa_2Cu_3O_{7-x}$ (123) ceramics in an interval of temperatures 875-975os was studied. The initial state with fine-grained equiaxial microstructure was received by a dynamic recrystallization during extrusion at 875os. It was established, that the growth of grains begins near 900os, that correlates with temperature of occurrence of liquid as a result of double (El) and threefold (E2) eutectics reactions. During annealing only plate-like grains initiate and grow, and the initial globular microstructure transfer to a lamella one. The kinetics of lengthening of plates does not undergo any changes in an interval of temperatures 900-975os. The average value of grain growth exponent (n) for the longitudinal size is close to 3. At the same time the kinetics of thickening of plates changes at all temperatures of annealing, and this change correlates with statistics of impingement of plates with each other. At the first stage of recrystallization, when plates grow almost independently from each other and impingements between them are rather seldom, the thickening of plates occurs at a rate less than for diffusion control. The change in the kinetics of thickening occurs at the moment of mass impingement of plates with each other. At the second stage of growth, when plates grow at conditions of competition with each other, the rate of plate thickening is close to diffusion control (W~tl/2) at all temperatures of annealing. The obtained data allows us to conclude, that growth of grains in 123 ceramics is Ostwald ripening of solid 123 grains in thin liquid matrix. The mean length of plates behaves similarly to the mean diameter of spherical particles, varying at Ostwald ripening by the normal cubic law. The value n=3 for the kinetics of lengthening of plates testifies that the lengthening of plates is controlled by diffusion through the liquid layer. In case of thickening the kinetics expected for the diffusion control realized only at the second stage of recrystallization. The change of the kinetics of plates thickening is analyzed within the framework of the step mechanism of growth of flat boundaries assuming that the main source of steps is joints of plates with each other.

(13) EFFECT OF COLD-ROLLED REDUCTION ON SECONDRY RECRYSTALLIZATION STABILITY IN GRAIN ORIENTED SILICON STEEL: MITSUMASA KUROSAWA[1]; Y. Hayakawa[1]; M. Komatsubara[1]; [1]Kawasaki Steel Corporation, Kawasaki Japan

Grain oriented silicon steel used for transformer-core material is usually classified into two types, CGO grades and HGO grades. HGO has better magnetic induction due to its higher alignment of secondary Goss grains. The amount of cold-rolled reduction is a main difference of them in manufacturing process, which typically applies 60% to CGO and 80% to HGO. The intermediate reduction rate in above range does not employ because of some secondary recrystallization instability during the final texture annealing. The major texture component of HGO, {111}<112>, increases withi ncreasing the amount of cold-rolled reduction, and would be helpful for the growth of secondary Goss grains. A question is why the intermediate reduction rate brings on the instability of secondary recrystallization. This work will focus on the texture change through a variety of the amounts of cold-rolled reduction to discuss stability of secondary recrystallization in this medium rate of reduction using extensive ODF analysis.

(14) COMPUTER SIMULATION OF THE DIFFUSION ACTIVATION ENERGY IN ZrO2 GRAIN BOUNDARY: Hualong Li[1]; Jerzy A Szpunar[1]; [1]McGill, Metallurgical Eng., 3610 University, Montreal, PQ H3A 2B2 Canada

Pressure tubes made of Zr-2.5% Nb alloys are used in the core of CANDU nuclear power reactors. During the operation, oxidation takes place. The oxide film, formed on the pressure tube surface, is a good barrier against oxidation and hydrogen ingress that can cause deleterious effect on the mechanical properties of the Zr-2.5% Nb alloy. In order to understand how and to what extent the oxide film protects the pressure tubes from the oxidation and prevents hydrogen ingress into metal, research has been carried on the diffusion processes through the oxide film. To simulate a role of grain boundary diffusion, sixteen CSL grain boundaries of oxide were constructed. The activation energies for oxygen self-diffusion along these grain boundaries were calculated using a potential of a central field repulsive potential plus a coulomb potential. The results are presented in the form of the activation energy of diffusion for oxygen in ZrO2 as a function of grain boundary misorientation angle and grain boundary axis.

(15) GRAIN GROWTH IN ELECTROEFINED VANADIUM: EDWARD A. LORIA[1]; [1]Metallurgical Consultant, 1828 Taper Drive, Pittsburgh, PA USA

Grain growth in the isothermal recrystallization of high-purity (electrorefined) vanadium has been studied as a function of annealing time, temperature and prior deformation. Specimens were cold rolled from 30 to 75 pct reduction in thickness then sealed in evacuated Vyear capsules and annealed between 700 and 1100ϒC for times up to 96 hr. The course of recrystallization was followed by means of hardness, metallographic and X-ray techniques. More than 30 pct reduction was necessary for recrystallization to occur at 850ϒC. With 60 pct reduction, it was initiated at 750ϒC and completed at 950ϒC. Grain growth was followed by determing, at room temperature, the average diameter of the same (largest) recrystallized grains in specimens annealed at 750 to 900ϒC. The average diameter of the five largest recrystallized grains at a particular time and temperature permitted the computing of the average rate of growth. The rates so determined are considered maxima. These average dimensions of the largest recrystallized grains were plotted vs. time, and growth rates were obtained from the slopes of the curves. Accordingly, the activation energy for grain growth was calculated at 75,000 cal per mole for the 750 to 900ϒC annealing range. Since the activation energy for grain growth was less than the 95,300 cal per mole for nucleation of recrystallized grains, the rate controlling factor in the recrystallization of vanadium must be nucleation.

(16) SIMULATIONS OF GRAIN GROWTH IN 2D BY THE STATISTICAL THEORY AND BY A DIRECT METHOD: R. BRANDT[1]; J. Svoboda[2]; K. Lücke[1]; [1]RWTH, Aachen Germany; [2]Czechoslovak

Academy of Sciences, Institute of Physical Metallurgy, Brno Czechoslovakia

The statistical theory of grain growth by Abbruzzese and Lücke considers the interplay of the physical requirement of grain boundary (GB) forces (determined by the number of sides) and the geometrical requirement of space filling. On the other side a direct numerical method for coarsening a 2D microstructure due to curvature driven grain boundary motion has been developed which allows to simulate an increase of areas up to a factor of 10 and the observation of all neighborhood relationships of interest. In particular it allows also to confirm the relationships describing the topological constraints used in the statistical theory. Results of simulation of normal grain growth by the statistical theory are compared to the results of simulations by the direct me thod. The foundations and the necessary suppositions of the statistical theory are checked and discussed with the help of such directly generated patterns.

(17) THE EFFECT OF GRAIN GROWTH IN THE PRESENCE OF STRONG TEXTURE ON THE GRAIN BOUNDARY NETWORK IN COPPER: O. V. MISHIN[1]; G. Gottstein[2]; [1]Riso National Laboratory, Materials Department, Roskilde DK-4000 Denmark; [2]RWTH Aachen, Institut für Metallkunde und Metallphysik, Aachen, Germany 52056

The effect of grain growth on grain boundary and triple junction distributions in strongly textured copper is investigated in this work. To stimulate grain growth, primary recrystallized copper with a strong recrystallization texture was successively annealed at different temperatures. Microstructural changes, evolution of texture and grain boundary ensembles during grain growth were investigated. Grain growth caused a strengthening of the recrystallization texture in pure copper. The impingement of cube oriented grains resulted in the appearance of many low-angle boundaries. Their fraction grew with increasing annealing temperature, whereas the frequency of high-angle CSL and random boundaries decreased. The changes in the crystallographic texture and grain boundary distribution reflected in the distribution of triple junctions. Slightly misoriented cube oriented grains clustered to form Σ1-Σ1-Σ1 triple junctions. Their fraction increased remarkably with the texture strengthening. The fraction of Σ3-Σ3-Σl junctions formed during grain growth at lower temperature remained constant upon additional high temperature annealing. The frequencies of triple junctions containing several random or special boundaries with Σ>3 tended to decrease during grain growth at higher annealing temperature.

(18) RELAXATION IN GRAIN GROWTH: TATSUZO NAGAI[1]; Kazuhiro Fuchizaki[2]; [1]Kyoritsu University, Physics Department, Kitakyushu 807 Japan; [2]Kyushu University, Department of Physics, Fukuoka 812 Japan

Relaxation to a scaling state in grain growth is investigated by computer simulation This relaxation has a hierarchical structure, i.e. after the average grain size first shows the l/2-power growth law the average grain shape relaxes slowly toward the scaling state. The latter is well described by the Kohlrausch anomalous relaxation law. Furthermore the relation of the slow relaxation to the elementary processes of topological change is discussed. We use the two-dimensional vertex model which describes the grain system as aggregation of vertices connected with each other by straight grain boundaries. The motion of vertices is determined by the balance equation between interface tension and friction force. Two elementary processes, the recombination (T1) and the triangle annihilation(T2), are further introduced to describe topological change of the system. We have carried out the simulation with the initial state of Voronoi pattern. As time goes on, each grain grows, shrinks or vanishes and then the whole system gradually coarsens toward the scaling state with the self-similar pattern. The mechanism of this relaxation phenomenon is elucidated.

(19) GRAIN BOUNDARY MIGRATION IN BICRYSTALLINE SAMPLES: O. B. NASELLO[1]; C. L. Di Prinzio[1]; [1]Ciudad Universitaria, Universidad Nacional de Cordoba, Facultad de Matermática Astronomia y Fisica, Cordoba 5000 Argentina

The different experimental methods currently used to study grain boundary migration in bicrystalline samples are analyzed. It is observed that they allow to determine Mγ, the product of the grain boundary mobility M and the grain boundary energy γ, only when the grain boundary is driven by a capillary force, which is independent of grain boundary inclination, and the interaction between grain boundary and sample surface is neglected. In a previous work (Di Prinzio et al., 1995) the motion equation of a grain boundary in a bicrystalline sample with the Sun and Bauer configuration was solved for anisotropic materials (ie those for which γ is a function of the grain boundary inclination). For the cases in which the grain boundary is dragged by the thermal groove formed at the intersection of the grain boundary with the sample surface, the movement was investigated only for some particular cases (Aristov et al, 1978; Mullins, 1958). In the present work the motion equation of grain boundaries in bicrystalline samples, with the different configurations presented in the literature, are solved in general. The grain boundary energy corresponding to anisotropic materials as well as the drag produced by thermal groove are considered. For each case, a discussion is presented regarding which of the intrinsic grain boundary parameters can be experimentally obtained.

(20) EFFECT OF NaCl ON GRAIN GROWTH IN ICE: L. ARENA[1]; O. B. Nasello[1]; [1]Universidad Nacional de Cordoba Ciudad Universitaria, Facultad de Matemátrica Astronomia y Fisica, Cordoba 5000 Argentina

In the present work grain growth in lO^{-6} NaCI doped ice is analyzed. The chosen concentration is similar to that observed in polar glacier ice. Polycrystalline samples are obtained by recrystallization of a single crystal. Samples are annealed at constant temperature in the range from -2 to -33ϒC for times that span up to 600 hs. Previous grain growth studies in NaCi doped ice, performed at higher concentrations and temperatures, indicated that, in ice, low concentration of impurities can increase grain boundary velocity. On the other hand, studies performed in polar glacier ice, at temperatures lower than -30ϒC, show that the impurities decrease the grain growth velocity. Preliminary results of this work suggest a different behavior of grain growth with annealing temperature.

(21) ON DESCRIPTION OF GRAIN GROWTH KINETICS: V. YU NOVIKOV[1]; [1]Moscow Institute of Steel and Alloys, Moscow Russia

It is commonly recognized that the equation D^2-D0^2=kt describes kinetics of normal grain growth provided all the grain boundaries are of identical properties and there is no pinning force or other constraining factors. Deviations from the dependence are usually considered as indication that the above-mentioned conditions are not fulfilled. Data on grain growth kinetics obtained by means of computer simulation on a series of model polycrystals having different initial microstructure are presented. It is shown that the above dependence fails to describe grain growth kinetics although all the above conditions are fulfilled. It is found that significantly better approximation of grain growth kinetics can be attained when the mean grain size, D, is substituted by the most probable grain size, Dm, i.e. Dm^2 Dm0^2=kt.

(22) THE LIFSHITZ-SLYOZOV STABILITY THEORY AND SIZE CORRELATION FUNCTIONS IN GRAIN GROWTH: P. STREITENBERGER[1]; [1]Inst fur Experimentl Physik, PSF4120, Magdeburg 00010 Germany

In the present paper the Lifshitz-Slyowv (LS) stability theory for the existence of a self-similar gram size distribution is formally generalized for an arbitrary cutoff grain radius P0 yielding an analytic expression for the size distribution function, which contains the cutoff radius as a free adjustable parameter. For each value of P0 within the interval ρ_{LS} ρ_o< × the size distribution automatically fulfils the LS stability conditions and reduces to Hillert's distribution for ρ_o =ρ_{LS} and to Louat's distribution in the limit ρ_o — × It is shown that the present generalization corresponds to the assumption of a specific size correlation between neighbouring grains, where the critical grain curvature is a linear function of the scaled grain radius. The two coefficients of this linear size correlation function are interrelated via their dependency on

the cutoff parameter ρ_o. Such linear size correlation functions have actually been found in recent computer simulations of one- and two-dimensional grain growth. By comparison with the present model it is shown how far such simulation results can be mapped onto a LS-like coarsening theory. The one-parameter fit of the present model yields grain size distributions which are in remarkable good agreement with the simulation results.

(23) THE COMPUTER MODEL OF RECRYSTALLIZATION TEXTURE IN INTERSTITIAL FREE STEEL: Y. HAYAKAWA[1]; J. A. Szpunar[2]; [1]Kawasaki Steel Corporation, Technical Research Laboratories, 1-Kawasakidouri, Mizushima, Kurashiki, Okayama 712 Japan; [2]McGill University, Department of Mining and Metallurgical Engineering, 3610 University Street, Montreal, Quebec H3A 2B2 Canada

Experimental work on automobile steels implies that the oriented nucleation mechanism plays the most important role in recrystallization texture development in IF steels. The cellular model of texture development in the stage of nucleation and growth of texture was proposed and verified by experiments. According to the proposed model the nucleation takes place in the vicinity of the grain boundaries and nuclei that are formed have orientation determined by the orientation of neighbouring grains. The nucleation starts at grains, that have the highest stored energy of deformation and then takes place at those grains that have lower stored energy. It was also assumed, that the probability of nucleation linearly decreases as the stored energy decreases. When the stage of nucleation is completed the neighbouring grains are consumed by the growing nuclei. No selective grain growth mechanism is imposed during the simulation, except that low angle grain boundaries are not mobile. The model presented is used to simulate experimental data describing texture nucleation and growth.

(24) MONTE CARLO SIMULATION OF GRAIN GROWTH ON ISOTROPIC LATTICES INFLUENCE OF A LATTICE STRUCTURE: M. Y. ALIES[1]; S. P. Kopisov[1]; A. Varnavsky[1]; [1]Institute of Applied Mechanics UBRAS, Izhevsk, Udmurt Republic 426001 Russia

The simulation of a microstructural evolution of a polycrystalline material with use of a Monte Carlo method and Potts model is well investigated and results obtained are in good correspondence with many experimental data of grain growth for polycrystalline materials. For simulation the anisotropic lattices were usually used, in two-dimensional it is a triangular and square lattices, in three-dimensional case it is a simple cubic lattice. Notwithstanding what the simulation on a triangular and square lattice shows essentially various evolution of a microstructure, not enough attention was given to influence of an initial discrete lattice structure, in particular its anisotropies. In offered paper the simulation of grain growth on isotropic lattices consisting from Voronoi polyhedrons in two and in three dimensions is considered, such approach allows to exclude influence of an anisotropy of a lattice. The calculations were performed for models with large number of allowed crystallographic orientations. In an outcome of simulation the normal grain growth was observed at T>0. The study of parameters of evolution of a microstructure shows the existence of a number of universal futures, in particular, exponential relation of mean growth rate from 1/T, constant energy of activation for an interval 0.3-0.8Tm, parabolic law of growth of the mean grain radius with temperature independent growth exponent value 0.5 on large times. The obtained statistical distributions and relations are in good correspondence with experimental data. The influence of a lattice structure on behavior and parameters of grain growth is considered at gradual recovery of a symmetry from isotropic distribution of Voronoi polyhedrons up to a correct six-coal lattice on a plane.

(25) SELF-ORGANIZED CLUSTERS OF MICROSTRUCTURE IN ZIRCONIA FILM: A. P. ZHILYAEV[1]; Jerzy Szpunar[1]; Valery Gertsman[1]; [1]McGill University, Department of Metallurgical Engineering, 3610 University Street, Montreal, Quebec H3A 2B2 Canada

HRTEM study (V.Y.Gertsman, Y.P.Lin, A.P.Zhilyaev and J.A.Szpunar, Phil. Mag. A (1997) submitted) was used to identify specific regions in the structure of the oxide layer grown on the surface of a zirconium alloy. Dimensions of those region are on the nanometer scale. The regions are built almost entirely of twins and appear as a maze pattern of rather regularly shaped crystallites with straight boundaries between them. Unlike material with the cubic lattice, several non-equivalent twin variants are possible in the monoclinic lattice of zirconia. Because of that, junctions consisting only of twin boundaries may exist in the monoclinic zirconia. This allows a unique situation which manifests itself a self-organized microstructures on the mesoscopic scale. The se microstructures have special properties. Being polycrystalline in nature, such areas behave with regard to diffusion processes almost as a single crystal. Computer simulation of the statistics of interfaces has been performed. The underlying idea in the modeling was a strong tendency to twin formation in zirconia when oxide layer is formed by oxidation of suitably oriented grains of alpha-zirconium. The grain boundary distributions obtained in such a way resemble that observed experimentally. Characteristic texture, created in the zirconia film, reflects certain orientation relationships between the crystal lattices of zirconia metal and its oxide.

(26) DEFORMATION PROCESSING, RECRYSTALLIZATION AND PROPERTIES OF MOLYBDENUM ALLOY: XU YOURONG[1]; [1]Shanghai, Jiading, Shanghai 201800 China

The extrusion, forging and sheet rolling for arc-cast Mo-0.5Ti alloy had been studied. Few dynamic recrystallizations can occur during high temperature extrusion at 1600°C, however, the coarse columnar grain of as-cast microstructure can be fragmented through the subsequent static recrystallization annealing at about 1400°C. The refined as-wrought microstructure can be progressively worked conveniently through forging and sheet rolling. The mechanical properties of sheet and piercing mandrel forging of Mo-0.5 Ti alloy also had been obtained. The behaviours of static recrystallization during high temperature deformation processing for as-cast and as-wrought Mo-0.5 Ti alloy also had been studied.

(27) DESIGN AND IMPLEMENTATION OF A DEDICATED MEASOSCALE INTERFACE MAPPING SYSTEM: W. YANG[1]; R. H. Rogan[1]; C. T. Wu[1]; M. DeGraef[1]; B. L. Adams[1]; [1]Carnegie Mellon University, Materials Science & Engr. Dept., Pittsburgh, PA 15213 USA

The determination of the grain boundary excess free energy as a function of misorientation over the entire fundamental zone requires the measurement of grain and boundary orientations at a large number of triple junctions. Serial sectioning methods can be used in combination with orientation imaging microscopy and atoms force microscopy to determine the geometric information needed to construct the energy function. In this contribution we will present a dedicated mesoscale interface mapping system, based on a Philips XL40 field emission SEM equipped with an OIM system. The system is capable of automatically locating triple junctions and acquiring electron backscattering patterns for all three grains meeting at the junction. We will discuss the implementation of an optimized Hough Transform and peak finding routine, band indexing (including band width information), triple junction detection algorithms, and 3D junction geometry analysis.

(28) MEASUREMENTS OF GRAIN BOUNDARY THERMAL GROOVES AS A FUNCTION OF ORIENTATION IN Al_2O_2 AND MgO: D. M. SAYLOR[1]; G. S. Rohrer[1]; [1]Carnegie Mellon University, Materials, Science & Engr. Dept., Pittsburgh, PA 15213 USA

The characteristic interfacial energies that provide the driving force for sintering and microstructure development in ceramic polycrystals can potentially be quantified through observations of physical phenomena such as the thermal grooving of grain boundaries and surface faceting. Atomic force microscopy (AFM) is a facile technique for the measurement of thermal groove geometries and facet morphologies of polycrystals. In this paper, we will describe our efforts to measure the properties of a large number of interfaces in alumina and magnesia ceramics by coupling topographic AFM data with orientation data generated by orientation imaging microscopy (OIM). The observation of isothermal grain boundary groove evolution in alumina allows us to determine the dominant atomic removal mechanism (surface diffu-

sion) and the mass transport rate (D = 1x 10-9cm2/s at 1400°C). Thermal groove dihedral angle distributions for both systems were also derived by AFM. The mean ratio of surface to grain boundary energy is 1.2 for both alumina and magnesia. Finally, based on OIM measurements of grain orientation, the crystallographic orientation dependence of the relative interfacial energies will be discussed.

(29) A SIMS CHARACTERIZATION OF BANDED MICROSTRUCTURES IN Ni-Cr-Fe ALLOYS: M. G. BURKE[1]; B. Z. Hyatt[1]; G. McMahon[1]; [1]Westinghouse Electric Corporation, Bettis Atomic Power Laboratory, West Mifflin, PA 15122 USA

The development of banded microstructures in Ni-Cr-Fe alloys, particularly Alloy 600, is generally associated with the presence of carbide bands in the material. Banded microstructures in Alloy 600 consist of coarse and fine-grained "bands" aligned parallel to the working direction. Heat treatments at temperatures in the range of 1050-1100°C will tend to dissolve carbides in these alloys. However, the presence of the banded carbides persists to elevated temperatures. The resultant fine-grained microstructures in these carbide-banded regions are due to the pinning of migrating grain boundaries during the annealing treatment. This study was undertaken to identify the microstructural and microchemical features that are associated with the development of the banded microstructures. To determine what elemental species were associated with the banded carbides, secondary ion mass spectroscopy (SIMS) analysis coupled with conventional microstructural characterization techniques was used to evaluate a series of heat-treated specimens of Alloy 600. The results of this study showed that the Cr-containing carbides within the banded fine-grained regions are enriched in boron. Boron was also detected at grain boundaries after elevated temperature solution-anneals. The resistance of these intragranular carbides to dissolution during the solution-anneal is associated with the incorporation of boron into the Cr-rich carbides in Alloy 600.

(30) SYMMETRIES OF THE GRAIN BOUNDARY DISTRIBUTIONS: A. MORAWIEC[1]; [1]Carnegie Mellon University, Dept. of Materials Science and Engineering, Pittsburgh, PA USA

The distribution of grain boundaries is necessary to perform statistical calculations on the boundaries in polycrystalline aggregates. Here, it is assumed to be a function of five macroscopic boundary parameters describing misorientation of grains and inclination of the boundary. Because of crystal symmetries the parameters are not unique, i.e., a number of different sets of parameters represent the same geometrical arrangement at the boundary. The distribution must take equal values for these arguments, and thus, it also exhibits certain symmetries. Its domain can be reduced to an asymmetric domain, i.e., to a part of the parameter space in which each physically distinct boundary is represented only once. This also concerns all other functions of similar nature assumed to depend on macroscopic parameters, e.g., grain boundary energy. For given symmetries of neighboring crystals, the problem is determining the symmetries of the grain boundary distribution and the shape of the asymmetric domain. Although the issue is relatively basic, we are unaware of any complete treatment of it in literature. Possible symmetries of distributions are investigated for both homo- and heterogeneous grain boundaries. Using the already known domains for misorientation distributions, the asymmetric domains of grain boundary distributions can be easily obtained. The solutions will be given for all possible combinations of crystallographic symmetries. Moreover, some other properties of the space of the macroscopic boundary parameters are considered.

(31) 3D MICROSTRUCTURE CHARACTERIZATION THROUGH SERIAL SECTIONS AND RECONSTRUCTION PROCESSES: C-C. YANG[1]; [1]Carnegie Mellon University, Department of Materials Science and Engineering, Pittsburgh, PA USA

Evolution of grain structure via grain growth leads to both increasing average grain size and changing grain orientations and misorientation distributions in the system. The large variation in the properties of grain boundaries with crystallographic character, including intrinsic variables such as grain boundary mobility and grain boundary energy, is the main factor which cause the change of texture and misorientation distributions during curvature-driven growth. In order to observe the real three-dimensional arrangement, distribution, and the morphology of grains inside a polycrystal sample system during grain growth, an acquisition technique which is based on serial sections and image reconstruction is described. The main focus will be on the extraction of geometrical parameters such as dihedral angles and boundary curvatures.

(32) WETTING OF Fe-Mn ALLOY GRAIN BOUNDARIES BY LIQUID Cu: M. TAKASHIMA[1]; [1]Carnegie Mellon University, Department of Materials Science and Engineering, Pittsburgh, PA USA

The effect of grain boundary character on grain boundary wetting by liquid copper has been investigated in an fcc Fe-30wt%Mn-10wt%Cu alloy. Cu films were found along some grain boundaries in the alloy after annealing (above the peritectic temperature) at 1120C, followed by quenching. The fraction of wet grain boundaries was low at both small (less than 20 degrees) and large (more than 50 degrees) misorientations, and high at intermediate misorientations. In particular, all sigma 3 grain boundaries were not wet. This indicates that lower grain boundary energy leads to a lower fraction of wet grain boundaries, as expected. In order to develop a more complete understanding of why certain small misorietation boundaries are wet, and why certain large misorientaion boundaries remain dry, the effects of the complete set of five degrees of freedom, which are needed to fully characterize a grain boundary, should be investigated.

(33) IMAGE PROCESSING FOR GRAIN BOUNDARY DETECTION IN MICROSCOPE IMAGES: A. TALUKDER[1]; D. Casasent[1]; S. Ozdemir[1]; [1]Carnegie Mellon University, Department of Electrical and Computer Engineering, Pittsburgh, PA USA

A new algorithm fusion approach using wavelet filters is used to detect grain boundaries with low contrast in the presence of noise. Imaginary and real Gabor wavelet filters are used at two scales and these are combined using algorithm fusion to locate grain boundaries with different properties (gray-scale transition grain boundaries and line grain boundaries) of various sizes (scales) under varying contrast and noise conditions. This novel algorithm fusion approach is tested on different microscopy images of several materials and shown to be robust to these changing imaging conditions. A real-time skeletonization approach is also used that applies a new and efficient hit and miss transform (HMT) to produce lines of one pixel width. A line following algorithm is implemented to locate triple junctions. Polynomial line-fitting techniques are used to estimate dihedral angles, and points where electron back-scatter pattern (EBSP) measurements should be taken on each grain are automatically located.

(34) THE LINK BETWEEN KINETICS AND CONFIGURATIONAL STATISTICS IN TWO DIMENSIONAL GRAIN GROWTH: COMPARISON OF THEORY AND SIMULATION: ANTHONY D ROLLETT[1]; ELIZABETH A. HOLM[2]; WILLIAM W MULLINS[1]; [1]Carnegie Mellon Univ., Materials Science & Engineering, 5000 Forbes, Pittsburgh, PA 15213-3890 USA; [2]Sandia National Labs., Physical & Joining Metallurgy, P. O. Box 5800, MS 0340, Albuquerque, NM 87185-0340 USA

Recent theoretical developments have shown that it is possible to make a quantitative link between kinetics of curvature-driven grain coarsening (in two dimensions) and the statistics of the quasi-steady state configuration. More specifically, the grain size distribution is determined jointly by the ratio of the (area) shrinkage rate of an isolated grain to the coarsening rate of a polycrystal together with the average number of sides of a grain as a function of grain size (relative to the mean radius). Slight deviations of the latter two quantities from the classical Hillert analysis lead to significant changes in the grain size distribution. All this information is readily available from simulations of grain growth. We have used a two dimensional Potts model with a square lattice to simulate grain growth. By application of the von Neumann-Mullins law to self-similar coarsening systems, we extract the kinetic ratio directly from the grain growth simulation results. The

distributions of size and number of sides are obtained by counting individual grains at regular time intervals. The results are compared to the theoretical analysis. Over a time interval in which self-similar coarsening holds for a reasonably large population of grains, the theory and simulations are in good agreement.

(35) THE ZENER EQUATION - A HISTORICAL OVERVIEW: M. FERRY[1]; [1]University of Wollongong, Department of Materials Engineering NSW 2522 Australia

The Zener equation was first reported by C. S. Smith in 1948 and since then has become an integral part of any theory which deals with recovery, recrystallization and grain growth in particle-containing materials. Several modifications to the original equation have been made over the past five decades to improve its applicability to more realistic situations. This paper summarizes and reviews these modifications and outlines possible future developments of the equation to predict the limiting grain size in particle-containing materials. The paper also examines the impact of the equation in the field of materials science and engineering.

(36) EVOLUTION OF 2D POTTS MODEL GRAIN MICROSTRUCTURES FROM AN INITIAL HILLERT SIZE DISTRIBUTION: C.C. Battaile[1]; E.A. Holm[1]; [1]Sandia National Laboratories, Albuquerque NM

The granular microstructure polycrystalline solids can affect a wide range of material properties including mechanical, thermal, optical, and electronic. Thus the properties of polycrystalline materials, and the mechanisms for grain formation and evolution, have been studied extensively for decades. In particular, normal grain growth in single-phase materials is relatively well understood. Simple analytical models, computer simulations, and experiments have all been used to characterize curvature-driven grain evolution. From these studies, the normal grain growth process is know to be self-similar, i.e., the normalized grain size distribution remains constant over time. Hillert performed an early analysis of this self-similar grain sizes. However, grain growth experiments and computer simulations exhibit self-similar grain size distributions that are not in agreement with Hillert's analysis. These experimental and simulated grain size distributions are much wider than the Hillert distribution, and are heavily skewed in the opposite direction. One proposed explanation for this discrepancy is that the simulations and experiments span an insufficient amount of time and thus do not represent the true self-similar grain size distribution. In order to examine this possibility, we performed 2D Potts Model grain growth simulations using topically realistic initial microstructure which have the Hillert size distribution. These initial microstructures were found to evolve away from the Hillert size distribution and toward that which has been observed previously in numerous studies.

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