MM 6: Interfaces II

Time: Monday 11:45–13:00 Location: H6

MM 6.1 Mon 11:45 H6

The role of quadruple points on grain microstructure evolution — •Volker Mohles, Luis Antonio Barrales-Mora, Lasar Shvindlerman, and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen, 52056 Aachen

It is well known that triple junctions between grains can have a significant influence on grain microstructure evolution. Now the effect of quadruple points on grain microstructure evolution has been investigated by computer simulations. For this purpose, a special grain assembly was employed. This special configuration allows a steady-state motion of the grain boundaries, permitting to study the effect of a finite mobility of the quadruple points on the evolution of the system. Numerous simulations, by means of a 3D Vertex Model, were performed varying the quadruple point mobility. The results of these simulations clearly demonstrate that quadruple points can drag grain growth kinetics. However, further simulations on the same configuration but for different triple junction mobilities showed that the dragging effect of triple junctions is considerably larger than the effect of quadruple points.

MM 6.2 Mon 12:00 H6

Bond-order potential for atomistic modeling of extended defects in tungsten — •Matous Mrovec[1,2], Christian Elsaesser[1,2], and Peter Gumbsch[1,2] — [1]IZBS, University of Karlsruhe, Kaiserstr. 12, 76131 Karlsruhe — [2]Fraunhofer-Institute IWM, Woehlerstr. 11, 79108 Freiburg

The bond-order potential (BOP) for transition metals is a real-space semi-empirical description of interactions between atoms, which is based on the tight-binding approximation and the d-band model. This scheme provides a direct bridge between the electronic-structure modeling and the atomistic modeling by coarse-graining the electronic degrees of freedom into a many-body interatomic potential. We will present a recently constructed BOP for the body-centered cubic transition metal tungsten. The potential was extensively tested against accurate DFT methods in order to assess its reliability and applicability. The high predictive power of the BOP will be demonstrated in studies of extended defects, namely low-index surfaces, symmetrical tilt grain boundaries, and lattice dislocations, which all affect the mechanical behavior of polycrystalline tungsten.

MM 6.3 Mon 12:15 H6

Untersuchung des Energie-Missorientierung-Phasenraums allgemeiner Cu-Korngrenzen — •Markus Ziehmer[1], Andreas Tschöpe[1], Carl Krill III[2] und Rainer Birringer[1] — [1]Technische Physik, Universität des Saarlandes, 66041 Saarbrücken — [2]Elektrotechnik, Universität Ulm, 89081 Ulm

Die spezifische Korngrenzenenergie γ ist von der Missorientierung $(\Theta,\vec{r})$ der angrenzenden Körner abhängig. Daraus resultiert ein Drehmoment, das unter der Voraussetzung ausreichender thermischer Aktivierungsenergie die Rotation der Körner in Richtung lokaler Energieminima antreibt.

Die Verbindung der etablierten Kugel-Platte-Methode mit der Orientierungsabbildenden Mikroskopie (OIM) bietet die Möglichkeit, die Rotation einzelner einkristalliner auf einem einkristallinen ebenen Substrat angesinterter Kugeln zu detektieren. Aus der Aufzeichnung der sich ändernden Missorientierung zwischen Kugel und Platte lassen sich Rückschlüsse über charakteristische Merkmale des $\gamma(\Theta,\vec{r})$-Phasenraums ziehen. Zusätzlich kann man unter der Annahme der Parallelität von Korngrenzenebene und Substratoberfläche die Tilt- und Twistanteile bestimmen.

Frühere Untersuchungen der Missorientierungsabhängigkeit von γ wurden meist an reinen Tilt- oder Twistkorngrenzen vorgenommen. Wir berichten über Messungen an allgemeinen Cu-Korngrenzen, die darauf hinweisen, dass die beobachteten Phänomene nicht durch das bisher verwendete einfache Bild des Energie-Missorientierung-Phasenraums adäquat beschrieben werden können.

MM 6.4 Mon 12:30 H6

Ab-initio based multiscale analysis of the 5D configurational space of Grain Boundaries in Aluminum. — •Liverios Lymperakis and Jörg Neugebauer — Computational Materials Design department, Max-Planck-Institut für Eisenforschung, Düsseldorf

A rapidly evolving approach in materials design is Grain Boundary (GB) engineering, i.e. optimizing the population of GBs with desirable geometry by suitable thermomechanical treatment. To achieve this, a deeper understanding and quantification of the interplay between the GB energies with respect to the misorientation of the two grains (3 dimensional configuration space) and the inclination of the boundary plane (2D space) are crucial. In this work we combine first principles density functional theory with modified embedded atom method (MEAM) calculations in order to explore the 5D-phase space of GBs in Aluminum. To handle this problem, we have generalized our implicit boundary multiscale schema (IBMS) which had been originally developed and applied to study isolated dislocations [1]. In a first step we have explored the three degrees of freedom required to describe the misorientation of the two grains: as an example we discuss symmetrical tilt GBs having the rotational axis along high symmetry directions of the fcc lattice. As a second example we focus on the low energy misorientation angles and explore the remaining two degrees of freedom associated with the inclination of the boundary plane. These results have been able to interpret and explain recent experimental data on GB occupation [2]. [1] L. Lymperakis et al. Phys. Rev. Lett. 93, 196401 (2004). [2] C.-S. Kim et al. Scripta Materialia 54, 1005 (2006).

MM 6.5 Mon 12:45 H6

Simulations of grain coarsening considering complex energy dependences — •Yingxiao Ma, Volker Mohles, Luis Antonio Barrales-Mora, and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen, 52056 Aachen

The energy of grain boundaries in metals depends on their geometrical parameters (misorientation and inclination) in a complex manner. A function is proposed which allows to describe this energy dependence in a rather convenient way for engineering purposes. It is based on the idea of special large angle boundaries (sigma boundaries) being superimposed with small angle boundaries, in order to describe general boundaries. The energy of the small angle part is derived from dislocation theory, whereas the high angle part may be derived from atomistic simulations. Applying this energy function, the 2D vertex dynamics model is used to simulate grain growth in Aluminium. Microstructure evolution, grain growth kinetics, the von Neumann-Mullins relation and the distributions of grain size and misorientation in 2D polycrystals have been examined. The sensitivity of the results on the initial conditions (experimental/random orientations) and on the details of the energy function is determined.