MM 46: Interfaces

Time: Thursday 16:30–18:15 Location: H 0111

MM 46.1 Thu 16:30 H 0111

Effect of the finite mobility the grain boundary junctions on the MacPherson-Srolovitz relation for the growth rate of polycrystalline systems — •Luis Antonio Barrales Mora[1], Volker Mohles[1], Lasar S. Shvindlerman[1,2], and Günter Gottstein[1] — [1]Institut für Metallkunde und Metallphysik, RWTH Aachen, Kopernikusstr. 14, D-52074 Aachen, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow District 142432, Russia

Recently, MacPherson and Srolovitz formulated the three-dimensional equivalent to the von Neumann-Mullins relation. In contrast with the latter, the new relation does not include directly the topological class of the grains but relates mainly to their metrics. Since a finite mobility of the boundary junctions (triple lines and quadruple junctions) affects the kinetics of the evolution of the granular system, repercussions in the MacPherson-Srolovitz relation are to be expected. In the present contribution, a three-dimensional vertex model is used in simple granular assemblies for the verification of this important relation. In addition, the effect of a finite mobility of the boundary junctions and its impact on the MacPherson-Srolovitz relation is analysed.

MM 46.2 Thu 16:45 H 0111

Mechanisch induzierte Bewegung der <100> Kippkorngrenzen in Al-Bikristallen — •Tatiana Gorkaya, Dmitri A. Molodov und Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen

Es wurde die Bewegung von planaren Korngrenzen, die durch eine angelegte Schubspannung induziert wurde, in Al-Bikristallen gemessen. Symmetrische <100> Kippkorngrenzen mit Rotationswinkeln im gesamten Desorientierungsbereich (0-90°) wurden dabei untersucht. Die Experimente zeigten ideale Kopplung zwischen der Korngrenzenbewegung in die Richtung normal zur Korngrenzenebene und der lateralen Verschiebung der Körner. Die gemessenen Verhältnisse zwischen denen stimmen perfekt mit der entsprechenden Korngrenzengeometrie überein. Weiterhin wurde ein Übergang von der Korngrenzenbewegung, die mit der Kornverschiebung gekoppelt ist, zum rigiden Kornabgleiten entlang der Korngrenzenebene beobachtet, der von der Temperatur, der angelegten Schubspannung und Korngrenzengeometrie abhängt. Die Experimente zeigten auch, dass sich die Korngrenzen mit θ bis etwa 30° und ab 60° in entgegengesetzte Richtungen bewegen. Für Großwinkelkorngrenzen mit θ im mittleren Winkelbereich (30°-60°) wurde die Korngrenzenbewegung in beide Richtungen, abhängig von experimentellen Parametern, beobachtet. Die Temperaturabhängigkeit der Korngrenzenbeweglichkeit wurde in einem Temperaturintervall zwischen 280 und 400°C gemessen und entsprechende Aktivierungsparameter der mechanisch induzierten Korngrenzenbewegung wurden bestimmt.

MM 46.3 Thu 17:00 H 0111

Simulation of partial melts with a phase-field model — Jens Becker[1], Britta Nestler[2], and •Frank Wendler[2] — [1]Institute of Geoscience, University of Tübingen, Sigwartstr. 10, 72076 Tübingen, Germany — [2]Institute of Computational Engineering, University of Applied Sciences Karlsruhe, Moltkestr. 30, 76133 Karlsruhe, Germany

Partially molten grain systems are of great interest in engineering (thixoforming, rheocasting) as well as in geology, as they appear in the rock forming layers of the deeper earth's crust. Particularly properties like the growth rate of isolated grains as well as coarsening in grain ensembles are substantially modified after partial melting. We present recent results found by applying our formerly introduced multi phase-field model (a diffuse interface method based on the formulation of a Ginzburg-Landau free energy functional) to partial melts. First, details on the phase-field model and the numerical aspects necessary to treat the enormous computational effort for a large grain system are presented. Secondly, a comparison of normal grain growth in 2D with grain growth in partial molten systems is given. The parabolic growth law and the validity of the von Neumann-Mullins relation for isolated grains are found to hold very well in the case of normal grain growth simulations. Partial melts in contrast show a strongly reduced growth rate. The dependancy on wetting angles, liquid fraction and permeability of the grain structure is highlighted using results in from 2D and 3D simulations. Additionally, the evolution of 'wet' triple points including an orientational dependancy of the surface energy are shown as a first step to clarify the role of anisotropy in partial melts.

MM 46.4 Thu 17:15 H 0111

ELNES at internal metal-oxide interfaces — •Oliver Heckl[1] and Ferdinand Haider[2] — [1]ETH Zürich, Institute of Quantum Electronics, Wolfgang-Pauli-Str. 16, 8093 Zürich — [2]University of Augsburg, Institute of Physics,Universitätsstr. 1 , 86135 Augsburg

The heterophase boundaries between precipitates such as spherical amorphous SiO_2 particles inside a copper matrix as well as crystalline CuO precipitates inside a silver matrix and the surrounding metal matrix are examined with high spatial resolution using a scanning transmission electron microscope (STEM) equipped with an electron energy loss spectrometer (EELS). Typical features of the electron energy loss near-edge fine structure (ELNES) of the oxygen K ionization edge allow to determine the bonding state of oxygen and thus to detect interlayers at the phase boundary. The validity of Kirchheim's structural vacancy model of oxygen segregation at metal-oxide interfaces is verified this way. It predicts that no interfacial accumulation of excess oxygen occurs at the phase boundary of amorphous precipitates. For the Ag-Cu alloy there is the additional degree of freedom for the oxidation value of copper and it can be seen that structural vacancies change the oxidation value at the phase boundary.

MM 46.5 Thu 17:30 H 0111

Ab-initio and atomistic simulation of interfaces in Aluminium — •Thomas Gnielka[1], Peter Gumbsch[1,2], Pim Schravendijk[2], and Christian Elsässer[2] — [1]IZBS, Universität Karlsruhe (TH), Kaiserstr. 12, 76131 Karlsruhe — [2]Fraunhofer IWM, Wöhlerstr. 11, 79108 Freiburg

Various macroscopic properties of polycrystalline materials originate from their microstructure, which itself depends on structural and chemical properties of extended defects (dislocations, grain and phase boundaries) at the atomic level. Therefore an important task for a scale-bridging modeling of polycrystalline materials is the coupling of different calculation methods at different size and time scales. In this talk an example for the combination of ab-initio calculations, based on the density functional theory (DFT), and atomistic simulations with empirical interatomic potentials will be addressed. While ab-initio DFT methods can calculate energies with high predictive power but for rather small systems, atomistic simulations with potentials validated with respect to first-principles results make it possible to study materials systems with thousands of atoms at a reasonable compromise of accuracy and efficiency. In this work grain boundaries in aluminum were studied as model systems, and first results for two pure boundaries will be presented and discussed.

MM 46.6 Thu 17:45 H 0111

Ab-initio investigation of chromium carbide - diamond interfaces — Andreas Böhner, •Rebecca Janisch, and Alexander Hartmaier — Friedrich-Alexander-University Erlangen-Nürnberg, Department of Materials Science and Engineering, Institute of General Materials Properties

Superhard carbon coatings, e.g. diamond like carbon on ductile tool steels, promise to feature exceptional resistance to frictional wear and corrosion. Therefore, the development of such carbon coatings is an active field of materials research. A crucial task is to optimize the adhesion between the carbon coating and the subjacent alloy.

To this end we perform a case study of the interface between diamond and chromium carbides of different stoichiometry. We use ab - initio density functional calculations employing plane waves and pseudopotentials. The first step is to study bulk properties - such as equilibrium lattice constant, bulk modulus, and details of the chemical bonding - of different chromium carbides. We then select certain phases for constructing supercells to model the CrC_x diamond interface. After relaxing macroscopic and microscopic degrees of freedom, these interfaces are characterized by calculations of the work of separation and investigation of the electronic structure at the boundary. The influence of superimposed stresses and strain on the results is discussed. The results show a systematic dependence of the characteristic quantities on the C concentration in the carbide and can explain different experimental observations.

MM 46.7 Thu 18:00 H 0111

Gaussian Polarizable Model for Metal Oxides — •Fawzi Mohamed and Joachim Sauer — Humboldt University

We present the first results of a polarizable force field geared toward metal oxides which is well suited for QM:MM embedding.

The model uses atom centered gaussians s and p functions to describe the long range electrostatic part.

The s function charge is assumed to be constant (no charge transfer allowed) and the p functions depend on the field and the local environment around each atom.

The optimal values for the s and p functions, the values that the potential tries to fit, are obtained from the electronic density ρ of DFT calculations minimizing

$$E = (\rho - \tilde{\rho}|\rho - \tilde{\rho}) = \int \frac{(\rho(r) - \tilde{\rho}(r))(\rho(r') - \tilde{\rho}(r'))}{|r - r'|} dr dr' \qquad (1)$$

as is done in RI methods, but only to reproduce the long range part of it. This is achieved by replacing the $1/|r - r'|$ operator with

$$C(r, r'')F(r'')C(r'', r) \qquad (2)$$

where C is half coulomb operator

$$\frac{1}{|r - r'|} = \int C(r, r'')C(r'', r')dr'' \qquad (3)$$

and F is a filter that removes the core region of the atoms.

Fitting these optimal values gives an implicitly interacting polarizable model that reproduces well the long range electrostatic field.

Then the short range part of the forcefield is optimized with force matching against DFT results.