MM 27: Interfaces I

Time: Wednesday 11:30–12:45 Location: IFW B

MM 27.1 Wed 11:30 IFW B

Grain boundary migration by molecular-dynamics simulation — •Jian Zhou, Volker Mohles, and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen, Aachen

Molecular dynamics simulations have been used to study grain-boundary migration of three series ([001], [011], [111]) of twist grain boundaries (GBs) in copper. An orientation-correlated force being able to drive flat GBs with different misorientations was applied to all twist GBs. The temperature dependence of the GB mobility was determined over a wide misorientation range. It is found that there is an obvious reduction in activation enthalpy with respect to GB migration when the temperature rises to a certain point for many high-angle and high-energy GBs. This reduction could be attributed to the structural change in GBs, such that different GB migration mechanisms become active. Moreover, GB structures were characterized by common neighbor analysis at low temperature. For low-angle GBs, a network of screw dislocations were traced, and it was found that this structure is relatively stable during the GB migration process. For high-angle GBs, in contrast, much more complicated and spatially extended GB structures were observed, which move mainly by a collective shuffle mechanism.

MM 27.2 Wed 11:45 IFW B

Phase-field modelling of foam microstructure evolution — •Frank Wendler, Eduard Stirner, and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences, Moltkestr. 30, 76133 Karlsruhe, Germany

Foam is a cellular materials with large variety of applications ranging from metal or polymer foams to cosmetics. After generation, a foam is a liquid with a complex rheological behaviour, dominated by surface free energy minimisation towards configurations of local equilibrium. We adapt a general multi phase-field model to describe this evolution step, important for the mechanical properties of a solidified foam material. Starting with a volume preserving Allen-Cahn model for incompressible dry foams with negligible liquid fraction (e.g. soap froth), a pressure dependant term is added to the functional of the free energy. This allows for the treatment of bubbles filled with a compressible gas. Assuming homogeneous pressures related to an equation of state a consistent model of boundary evolution can be given. The results approve that pressures within single bubbles are related to interface curvature according to the Young-Laplace equation. Simulations of bubble clusters and foam structures in 2D and 3D are presented, including the examination of pressure variations as a process step to optimize structure and accelerate equilibration. Finally, the treatment of wet foams with a non-negligible fraction of liquid, concentrated along the Plateau borders is given. Numerical evaluation of surface energies and dynamics show that it is not necessary to completely resolve the diffuse interface, which enables the simulation on larger length scales.

MM 27.3 Wed 12:00 IFW B

Simulations of surface energy driven processes at structured substrates — •Marcus Jainta and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences

We introduce a new method based on a phase-field model to simulate the behaviour of multiple phase regions at given non-moving obstacles with sharp interfaces in terms of new boundary conditions. We discuss the results for different surface energies of the simulated microstructures and bubbles. In addition, we consider adhesion forces in the presence and absence of fluid flow. The simulation results of liquid droplets on structured surfaces are compared with experiments related to the Lotus effect. Finally we discuss the numerical method and implementation of the new boundary conditions.

MM 27.4 Wed 12:15 IFW B

3D Vertex Dynamics Simulation of Grain Growth in Ceramics Including the Anisotropy of Grain Boundary Energy — •Melanie Syha[1], Ling Yue[1], Daniel Weygand[1], and Peter Gumbsch[1,2] — [1]Universität Karlsruhe, Institut für Zuverlässigkeit von Bauteilen und Systemen — [2]Fraunhofer IWM, Freiburg

A three dimensional (3D) vertex dynamics model for grain growth is presented, adapted to the study of grain growth in Strontium-Titanate-Oxide (STO) ceramics. The 3D vertex dynamics model for grain growth is an interface tracking model [1]. In this approach grain boundaries (GB) are discretized and their time evolution is derived from the minimization of the GB energy, which is dissipated by the motion of the GBs and triple lines. The original model [1,2] has been extended to handle misorientation and inclination dependent GB energies, mobilities and triple line drag. The improved model is compared to the 3D analogue of the Neumann-Mullins law [3].

The influence of structure dependent GB properties on statistical observables, e.g. grain size distribution function, grain growth dynamics and correlation function between grain size and number of neighboring grains is investigated. Cross sections through the grain structures are analyzed and compared to experimental observations on grain growth in STO ceramics

[1] D. Weygand, Y. Bréchet, J. Lépinoux, and W. Gust, Phil. Mag. B 79 (1999) 703. [2] D. Weygand, Y. Bréchet and J. Lépinoux, Interface Science 7 (1999) 285. [3] R. MacPherson and D. Srolovitz, Nature 446 (2007) 1053

MM 27.5 Wed 12:30 IFW B

THE FINITE MOBILITY OF THE BOUNDARY JUNCTIONS AND THE THEORETICAL PREDICTIONS OF GROWTH RATE FOR POLYCRYSTALS UNDERGOING GRAIN GROWTH — •Luis Barrales-Mora — Institut für Metallkunde und Metallphysik, RWTH-Aachen, Aachen, Germany

As a consequence of the recent demonstration of the three-dimensional von Neumann-Mullins relationship by MacPherson and Srolovitz, there has been a renewed interest in the investigation of the phenomenon known as grain growth. This interest arises from the many possibilities that this new relationship offers but also, and contradictorily, from its limitations. One of such limitations is the impossibility of this relationship to predict correctly the volume rate of change of grains if the motion of the grain boundaries is hindered. It is well known that many factors can hinder the grain boundary motion, e.g., second-phase particles, impurity atoms, the finite mobility of the boundary junctions, etc. In the present contribution, the latter factor is analysed in light of the Cahn-MacPherson-Srolovitz relationship by means of computer simulations. This relationship is coupled with theories on the finite mobility of triple lines and quadruple junctions and compared with simulation results in single grains. Similar relationships by Glicksman and Rios and Hilgenfeldt et al. are also investigated. This last point is relevant since these approaches allow the study of grain growth from a more statistical point of view.