DY 10: Growth processes and surface properties

Time: Monday 16:30–17:45 Location: H5

DY 10.1 Mon 16:30 H5

Phase Field Crystal Modeling of Dry and Wet Grain Boundaries — •Jesper Mellenthin[1], Alain Karma[2], and Mathis Plapp[1] — [1]Laboratoire de Physique de la Matière Condensée, École Polytechnique, 91128 Palaiseau, France — [2]Physics Department, Northeastern University, Boston, MA 02115 USA

The phase field crystal model has emerged as a powerful tool to simulate microstructural evolution in polycrystalline materials under a variety of nonequilibrium conditions. The crystal is represented by a local-time-averaged density field $\psi(\vec{r},t)$, which has the same symmetry as the crystalline structure. This density field is obtained by minimizing a free energy functional, which also allows for a second phase of constant ψ (a liquid phase) and coexistence between the two phases. The model naturally includes the elastic energy and the symmetry properties of the crystal and is therefore a convenient choice to investigate grain boundary properties.

In this work, we explore the influence of the misorientation between two crystals on the grain boundary structure. Dry grain boundaries become wet when the misorientation exceeds some threshold, in which case it becomes energetically favorable for a thin liquid film to exist between the two crystals. This produces an effective repulsion between the two solid-liquid interfaces that coalesce at a temperature below the normal melting point of a bulk crystal. Wet and dry grain boundaries are analyzed numerically and interpreted in the framework of phenomenological models for grain boundary structure.

DY 10.2 Mon 16:45 H5

Relevance of surface viscous flow, surface diffusion and ballistic effects in keV ion smoothing of amorphous surfaces — •Sebastian Vauth and S. G. Mayr — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Amorphous metal or semiconductor thin films often show a dramatic smoothing reaction, when appropriately bombarded with keV heavy ions. Surface diffusion, surface viscous flow and ballistic effects have been suggested as possible candidates for the dominant atomic-scale smoothing mechanism. In the present study we compare the relative relevance of these processes by employing multiscale modeling, viz. a combination of molecular dynamics (MD) and continuum rate equations. This is achieved by deriving continuum expressions for a coarse-grained picture and calculating the corresponding coefficients from MD simulations. For this purpose diffusion constants, viscosities and lateral transport due to momentum transfer are evaluated. We observe the dominance of surface viscous flow over surface diffusion for any surface morphology while ballistic smoothing dominates for structures above a certain size threshold. These results are found to be valid for both, strong and fragile glasses, as represented by amorphous Si and CuTi.

This work is financially supported by the DFG Sonderforschungsbereich 602, TP B3.

DY 10.3 Mon 17:00 H5

Dynamics of steps on vicinal surfaces: Step-step interactions, sublimation and the Schwoebel effect — •Marian Ivanov, Vladislav Popkov, and Joachim Krug — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str.77, D-50937 Köln

Using morphological instabilities one can produce templates for nanoscale technology. One example of such an instability is step bunching, which splits a regular vicinal surface into regions of low and high density of monoatomic steps. The dynamics of the surface is described by the Burton-Cabrera-Frank model with boundary conditions provided by mass conservation at the steps. The instability condition can be found by linear analysis of the equations. For the case of pure sublimation with step-step interactions and Schwoebel effect, a new term arises in comparison to earlier calculations. In the continuum limit this leads to a restriction for the maximum bunch slope and to novel scaling properties for sufficiently large bunches.

DY 10.4 Mon 17:15 H5

Submonolayer growth of binary alloys — •Mario Einax[1], Sonja Ziehm[2], Wolfgang Dieterich[2], and Philipp Maass[1] — [1]Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau — [2]Fachbereich Physik, Universität Konstanz, 78457 Konstanz

We investigate the submonolayer growth of binary alloys, formed by co-deposition of A- and B atoms on a flat substrate. The dependence of the number densities of stable islands is determined as a function of incoming fluxes, adatom diffusion coefficients and binding energies of A and B atoms. Based on a generalization of mean-field rate equation theory novel scaling relations are predicted, which are in good agreement with kinetic Monte Carlo simulations of the growth process. Suggestions are made how to test the new theoretical predictions in experiments.

DY 10.5 Mon 17:30 H5

Rigorous selection theory for crystal growth with nonlinear transport — •Thomas Fischaleck and Klaus Kassner — Institut für Theoretische Physik, Otto von Guericke Universität Magdeburg, Postfach 4120, D-39016 Magdeburg

Asymptotic matching in the complex plane is a strategy for calculating exponentially small terms that has been pioneered for nonlinear equations by Kruskal and Segur. The method has been successfully applied to pattern-forming systems that could be cast into the form of a single ordinary differential or differential-integral equation. Examples are viscous fingering, dendritic crystal growth, or capillary water waves. Interestig problems that are modeled by nonlinear field equations with free boundaries, however, remained untractable.

We show how to combine asymptotic matching in the complex plane with Zauderer's decomposition scheme of nonlinear partial differential equations to study this class of problems. The method is exemplified by dendritic growth limited by nonlinear heat transport.