Overview:

Interfaces of condensed matter systems are essential for tooling the material properties and consequently that of derived devices and products in a whole range of applications from everyday household goods to opto-electronics and even further to medicine. Prominent examples are corrosion resistant surfaces of household goods, or likewise noble surfaces of engineering protheses in medical applications. Thus there has been strongly increased effort in developing computational tools to support the understanding and to derive new design concepts for interfaces and surfaces of condensed matter systems during their processing to a materials system. This comes along with an inherent multi-scale challenge due to the large range of time- and length scales on which essential physical and chemical mechanisms occur. Here we present three examples as a representative cross-section of our model portfolio in this topic.

Phase-Field-Crystal / Phase-Field Method:

Homogeneous nucleation is a part of many solidification processes, and phase-field models are capable of describing via the addition of noise terms. However, it is hard to adjust the noise parameters of phase-field simulations to experimentally determined nucleation rates. Phase-field crystal (PFC) simulations are capable of efficiently simulating homogeneous nucleation on the atomic scale (a), and by adjusting the noise amplitude $G$ it is possible to determine different nucleation rate regimes (b) and ultimately compare them with experimental data to determine noise parameters for phase-field simulations of nucleation processes, which capture appropriately the thermal activation of the system.

Selected references:
- J. Hubert, M. Cheng, H. Emmerich. Effect of noise-induced nucleation on grain size distribution studied via the phase-field-crystal method. JPCM (2008), in press.

Phase-field/Monte-Carlo hybrid algorithm:

A Phase-field/Monte-Carlo hybrid algorithm for the simulation of solutal growth of organic crystals is subsequently used for an investigation of diffusion effects. This method combines a two-scale phase-field model of liquid phase epitaxial growth and a Monte-Carlo algorithm of the 2D nucleation. It is considerably faster than previous pure Monte Carlo simulations of crystal growth. The study of diffusion effects is carried out based on an example of a hydroquinone crystal, which grows from water solution at various supersaturations. The dependencies of the growth rate and the nucleation rate on the supersaturation indicate the change of the growth mechanism from spiral growth to 2D nucleation (see Fig.). The difference in the growth rate for various faces is in agreement with the crystal morphologies derived from the attachment energy method and those observed experimentally. The main result of our simulations is the evaluation of engineering limits to choose optimal process conditions.

Selected references:

Phase-field simulation of microstructure solidification of Fe-Mn alloy under the influence of forced convection:

In this work we have extended a quantitative phase-field approach to simulate dendritic growth of a Fe-9.8mol%Mn alloy under the influence of an imposed flow field. We show the influence of (macroscopic) convection on growth in peritectic material systems, Philosophical Magazine Letters 87, 829 (2007).

Selected references: