MM 35: Topical Session Heterogeneous Nucleation I

Time: Thursday 11:00–13:00 Location: IFW D

Topical Talk MM 35.1 Thu 11:00 IFW D

On selected methodological challenges at the interface between quantum-mechanical approaches and phase-field modeling methods in computational materials science — •Martin Friak[1], Li-Fang Zhu[1], Alexey Dick[1], Alexander Udyansky[1], Johann von Pezold[1], Heike Emmerich[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Universität Bayreuth, Bayreuth, Germany

In order to reliably describe complex materials-science phenomena that are often bridging multiple length and time scales, different methods must be effectively combined. Achieving a seamless methodological interface between fundamentally different approaches still presents a major challenge despite of systematic and long-standing efforts. For the theoretical study of microstructural processes in multi-component and multi-phase metallic alloys considered here, a combination of quantum mechanical calculations and phase-field modeling constitutes the method of choice. In particular, the transferrability of quantum mechanical calculations ensures the predictive power of the approach, while the phase field model extends the accessible length and time scales in our simulations. The talk will critically review selected problems arising when ab initio calculations and/or atomistic simulations are employed to parametrise phase-field models for (i) the evaluation of the temperature dependence of thermodynamic, structural and elastic properties of different phases, (ii) the prediction of diffusion parameters, as well as (iii) the description of solid/liquid and solid/liquid interfaces.

MM 35.2 Thu 11:30 IFW D

Scale-Bridging Simulation on Atomistic and Mesoscopic Length Scales. — •Marco Berghoff[1] and Britta Nestler[1,2] — [1]Institute of Materials and Processes, Hochschule Karlsruhe, Germany — [2]Institute for Reliability of Components and Systems, Karlsruhe Institute of Technology (KIT), Germany

In the present analysis we study the process of early stage solidification using molecular dynamics (MD), phase-field crystal (PFC) and the phase-field (PF) methods. While the MD and the PFC methods are mostly in use at the atomistic scale, the PF can make meaningful predictions at the mesoscale. To demonstrate the ability of the PF in applications at the atomistic scale, we conduct a comparative study of growth of pure Ni in the early stage of solidification between MD and PF simulations. For this, the discrete atomic positions from the MD simulations are converted to a continuous field of the PF order parameter differentiating the phases, using the q_6q_6 operation. In addition, we tailor the parameters in the PF model to match those used in the MD model with a temperature dependent specific heat capacity and latent heat. We then compare the volume change of the nucleus as a function of time occurring in both simulation methods. As a substitute to MD simulations, we also used the PFC method for generating data at the atomistic scale, and compared the results with PF simulations. The ultimate goal is to benchmark the atomistic simulations with the PF method at the smaller scale and thereafter conduct PF simulations at the mesoscale, which is outside the realm of atomistic simulation methods.

MM 35.3 Thu 11:45 IFW D

Crystal growth, solid-liquid interfaces and nucleation in simple model systems: Computer simulations of Nickel — Roberto E. Rozas and •Jürgen Horbach — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany

Molecular dynamics as well as Monte Carlo simulation techniques are used to investigate crystal growth, solid-liquid interfaces and nucleation in Nickel. To determine various interfacial properties, inhomogeneous systems are prepared where the crystal phase at different orientations coexists with the fluid phase, separated by planar interfaces. Interfacial stiffness and tension are estimated using different predictions of capillary wave theory with respect to the capillary wave spectrum, finite-size broadening of the interfacial width and different geometries of the interface. Free energy barriers for the formation of a nucleus from the melt are computed via Monte Carlo simulation in conjunction with umbrella sampling techniques. Good agreement with recent experiments on Ni is obtained.

MM 35.4 Thu 12:00 IFW D

Phase-field simulations of inoculation and subsequent peritectic solidification in Ti-Al-B — •Markus Apel, Janin Eiken, and Ulrike Hecht — Access, RWTH Aachen

In Ti-Al based alloys boride particles can be used as grain refiners. By varying the B content in the melt, the formation temperature of boride particles can be adjusted in a way that they act as heterogenous nucleation sites for either the properitectic β- or the peritectic α-phase. We elucidate the effect of borides on microstructure formation by phase-field simulations coupled to a thermodynamic database. Nucleation and growth of small boride particles are explicitly taken into account on a scale below the numerical phase-field interface thickness by using a semi-analytical growth model. The simulation results show a variety of effects: grain refinement due to heterogeneous nucleation on TiB2-particles, interactions between the growing Ti phases and the borides, as well as a pronounced dependency of the phase transformation rates on the dominant nucleation sites.

MM 35.5 Thu 12:15 IFW D

growth of a two-phase finger in eutectic systems — •Guillaume Boussinot[1,2], Claas Hueter[1,2], and Efim Brener[1] — [1]forschungszentrum juelich — [2]MPIE duesseldorf

We present a theoretical study of the growth of a two-phase finger in eutectic systems. This pattern was observed experimentally by Akamatsu et al., Phys. Rev. E 61, 3757 (2000). We study this two-phase finger using a boundary-integral formulation and we complement our investigation by a phase-field validation of the stability of the pattern. The deviation from the eutectic temperature and from the eutectic concentration provide two independent control parameters, leading to very different patterns depending on their relative importance. We propose scaling laws for the velocity and the different length scales of the pattern.

MM 35.6 Thu 12:30 IFW D

Dendritic solidification along liquid-liquid interfaces — •Claas Hüter[1,2], Guillaume Boussinot[1,2], Efim Brener[2], Dimitri Temkin[2], and Robert Spatschek[2] — [1]MPIE, Düsseldorf — [2]Forschungszentrum Jülich

Solidification of an asymmetric dendrite along the interface of two liquids is discussed. The considered system shows a monotectic reaction, the diffusion equations and the associated thermodynamic boundary conditions are represented by three coupled nonlinear integral equations. The selection in this case determines the velocity, the lengthscale of the parabolic asymptotics of the dendrite and the lengthscale which defines the liquid-liquid interface. These quantities are determined as functions of the undercooling numerically.

MM 35.7 Thu 12:45 IFW D

Experimental determination of nucleation rates — •Joachim Bokeloh and Gerhard Wilde — Institut für Materialphysik, WWU Münster

Upon cooling a metallic melt, the nucleation rate changes from practically zero to virtually infinite in the small range of accessible crystallization temperatures, thus leaving only a narrow temperature window for experimental as well as for computational investigations. Both, the system size and the time scale of computational studies differ from those within reach of experimental studies by several orders of magnitude. Thus, for a meaningful comparison of computational and experimental works, the nucleation rates have to be extrapolated over several orders of magnitude. For this procedure, an accurate coverage of the nucleation rate over the complete accessible range is imperative. We present here data on the liquid undercooling behavior of Nickel obtained by repeated melting and crystallization in a DTA. This method allows acquiring a statistically meaningful data set under clean and reproducible conditions, from which nucleation rates can be determined. Supported by a variation of the sample mass from 10μg to 60 mg and classical isothermal nucleation rate measurements, the nucleation rate of pure Nickel was determined experimentally over a range of eight orders of magnitude and a temperature window of 70 K, thus allowing a true quantitative testing of the classical nucleation theory. Nickel was chosen as a model system because it shows high levels of undercooling and a well refined embedded atom potential is available for concurrent simulations.