MM 26: Computational Materials Modelling - Diffusion & Kinetics I

Time: Tuesday 15:00–16:00 Location: H24

MM 26.1 Tue 15:00 H24

Studying the kinetics of solid-liquid interfaces using transition path sampling — •Daniel Sopu, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

The properties of solid-liquid interfaces such as interface energies, interface mobilities and their anisotropy, play an important role in solidification theory. In a first-order phase transformation these interfacial properties determine to a large extent nucleation barriers and growth rates. Depending on the height of the nucleation barrier and the applied driving force, the solidification process can take place on extended time scales which makes it very inefficient to be studied using regular molecular dynamics. Here, we use transition path sampling (TPS) to study the solid-liquid phase transformation in a Lennard-Jones system. TPS is a rare event technique that creates an ensemble of reaction trajectories between two metastable states in phase space. By re-weighting the path ensemble we extract thermodynamic and kinetic properties of the transition and explore the transition mechanisms. In particular we investigate interface free energies, the nucleation and formation of the solid-liquid interface, and anisotropic interface mobilities as a function of temperature.

MM 26.2 Tue 15:15 H24

Effect of local ordering in the melt and at the solid-liquid interface on the growth kinetics in a metallic alloy model — •Mohammed Guerdane[1], Helmar Teichler[2], and Britta Nestler[1,3] — [1]Institute of applied Materials (IAM-ZBS), Karlsruhe Institute of Technology (KIT) — [2]Institute for Materials Physics, University of Göttingen — [3]Institute of Materials and Processes, Karlsruhe University of Applied Sciences

We present a molecular dynamics (MD) study about the structure of a solid-liquid interface between a bcc Zr crystal and a binary NiZr melt. We demonstrate how local atomic order in the liquid phase could transform into a massive lateral ordering at the interface when commensurability is given between the coordination polyhedra of the liquid and the periodic potential of the crystal wall. The influence of this structure on the growth kinetics is quantitatively investigated by linking MD simulations to phase-field modeling. These results contribute to our understanding of the correlation between the stability of the undercooled liquid against crystallization (e.g. in the case of glass forming alloys) and its ability to build up a pronounced atomic order.

MM 26.3 Tue 15:30 H24

Three-dimensional self-learning kinetic Monte Carlo — •Andreas Latz, Lothar Brendel, and Dietrich E. Wolf — Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, Duisburg, Germany

The reliability of kinetic Monte Carlo (KMC) simulations depends on accurate transition rates. The self-learning KMC method (Trushin et al 2005 Phys. Rev. B 72 115401) combines the accuracy of rates calculated from a realistic potential with the efficiency of a rate catalog, using a pattern recognition scheme.

We expanded the original two-dimensional method to three dimensions (Latz et al 2012 J. Phys.: Condens. Matter 24 485005). Excessive on-the-fly calculations of rates can be avoided by setting up an initial database, which can be done perfectly in parallel.

The performance is illustrated by applying the method to homoepitaxial growth of Ag on Ag(111) at low temperatures.

MM 26.4 Tue 15:45 H24

Electronic properties and diffusion behavior of Re in Ni-based superalloys: a combined DFT+kMC approach — •Sergej Schuwalow, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

High-temperature mechanical properties of Ni-based superalloys can be significantly improved by adding refractory alloying elements, such as Re, Mo or W. However, due to the complexity of the interplay between composition and microstructure the effect of these additives is only understood in a phenomenological way. Within this work, we investigate the diffusion and segregation behavior of alloying elements in Ni-based superalloys using a combination of *ab-initio* DFT calculations and kinetic Monte Carlo (kMC) modeling, with a particular focus on Re and its interplay with the γ/γ' phase interface. Re is known to be one of the slowest-diffusing elements in Ni [1], and is one of the most effective, and expensive, alloying additives currently in use. In this combined approach, DFT provides insights into local electronic properties of the γ/γ' interface and Re substitutional defects as well as into energetics of microscopic diffusion processes. Based on DFT data, a kMC model is developed to analyze diffusion and segregation behavior of alloying elements on an extended time scale.

[1] M. S. A. Karunaratne, P. Carter, R. C. Reed, Mat. Sci. Eng. A 281, 229 (2000)