MM 44: Invited talk Rogal

Time: Wednesday 19:00–19:30 Location: TC 006

Invited Talk MM 44.1 Wed 19:00 TC 006

Modelling solid-solid phase transformations: Atomistic insight on mechanisms and interface properties — •Jutta Rogal — Ruhr-Universität Bochum, Bochum, Germany

Atomistic modelling of the dynamics of phase transformations is a particularly challenging task. If the mechanism of the phase transformation is governed by so-called rare events then the time scale of interest will reach far beyond the capabilities of regular molecular dynamics simulations.

The atomistic rearrangements during solid-solid phase transformations in bulk systems involve massive structural changes including concerted multi-atom processes. The interface between two structurally different phases leads to a complex energy landscape that needs to be explored during the dynamical evolution of the interface. Here, we employ an adaptive kinetic Monte Carlo (AKMC) approach to investigate such processes at the interface between cubic and topologically close-packed phases in transition metals.

In particular we investigate the transformation between BCC and A15 in molybdenum. During the dynamical simulations a finite, disordered interface region evolves to compensate the structural mismatch between the two crystal phases. This disordered interface region makes the identification of a single transformation mechanism difficult. Still, from our simulations we extract a rate for the layer transformation which we relate to an effective barrier for the transformation mechanism and discuss the corresponding atomistic processes that we find along the transformation path.