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Enhanced sampling approaches to capture atomistic processes during structural phase transformations in condensed matter systems

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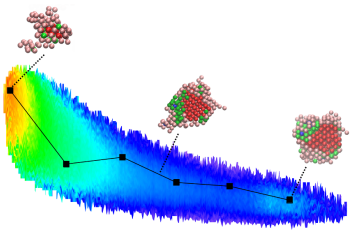

Obtaining atomistic insight into the fundamental processes during structural phase transformations and their dynamical evolution up to experimental timescales remains one of the great challenges in materials modelling. In particular, if the mechanisms of the phase transformations are governed by so-called rare events, the timescales of interest will reach far beyond the applicability of regular molecular dynamics simulations. In addition to the timescale problem the simulations provide a vast amount of data within the high-dimensional phase space. A meaningful physical interpretation of these data requires the projection into a low-dimensional space and the identification of suitable reaction coordinates.

In this presentation, I will give an overview of our recent progress in the application of advanced atomistic simulation techniques to capture the dynamical behaviour during phase transformations over a large range of timescales. One of the key results is the analysis of nucleation and growth mechanisms during solidification in metals that can be extracted from transition path sampling simulations. By applying a likelihood maximisation scheme the quality of different reaction coordinates is evaluated which enables us to identify the most important order parameters that characterise the atomistic processes during the initial stages of nucleation and growth. A second example is the analysis of phase boundary migration during a solid-solid transformation in molybdenum between the topologically close-packed A15 and the body-centred cubic phase. The transformation proceeds via collective displacements of atoms in the interface region. The associated effective energy barrier that determines the mobility of the phase boundary is not associated with specific atomistic processes, but results from the characteristic features of the complex energy landscape that the system explores during the transformation.

Einführung: Prof. Dr. R. Drautz

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