INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Seminar

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Kinetic Monte Carlo simulations of decomposition in Fe-Cr alloys

Phenomenological descriptions of diffusive phase transformations in alloys are often limited by the complexity of the thermodynamic and kinetic properties of real systems, which are difficult to describe precisely at the macroscopic scale. At the atomic scale however, complex kinetic behaviours arise out of simple diffusion mechanisms that usually involve point defects. The atomic modelling of the transformation therefore requires a good description of the diffusion events, i.e. of the point defect concentrations and jump frequencies, and the way they depend on the local atomic environment. Atomistic Kinetic Monte Carlo (AKMC) simulations based on rigid lattice approximations are used to model the diffusion mechanisms. They are especially efficient when the key parameters of the model are computed by ab initio calculations. We present here such Monte Carlo simulations of α-α' decomposition in iron-chromium alloys, during thermal ageing and under irradiation. They are compared with experimental studies (by 3D atom probe and small-angle neutron scattering measurements). The effects of the ferro-to-paramagnetic transition on the kinetics of decomposition are considered.