INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

The ICAMS Seminar presents

Dr.-Ing. Oliver Kastner
Ruhr Universität Bochum
Fakultät Maschinenbau, Institut für Werkstoffe

Monday, 20th of April, 4 p.m.
ICAMS Seminar room UHW 11/1102

Principle investigation of martensitic transformations in 2D Lennard-Jones crystals

Binary Lennard-Jones crystals may serve as a test system to study austenite/ martensite lattice transformations. We present results of a 2D molecular-dynamics principle investigation. In 2D, nested square lattices (the model austenite) may undergo transitions into nested hexagonal lattices (the model martensite) in both temperature and load control mode. The model material shows full thermo-mechanical coupling and thus is capable of related material behaviour (pseudo-plasticity/ elasticity, shape memory effect). A rich transformation morphology can be studied even in 2D. Among the observed phenomena we show the propagation of travelling transformation fronts, martensitic plate growth, the twinning process, the formation/ accommodation of martensitic domain structures, the generation of transformation-related lattice defects and their influence on cyclic loading processes.

One interesting result is that the model material forms coherent, finite-sized martensitic twin-structures in absence of twin/ twin interface energies. The formation of such microstructure is originated by the transformation dynamics on the mesoscopic level of length scale.