Microstructure formation and hysteresis in shape memory alloys

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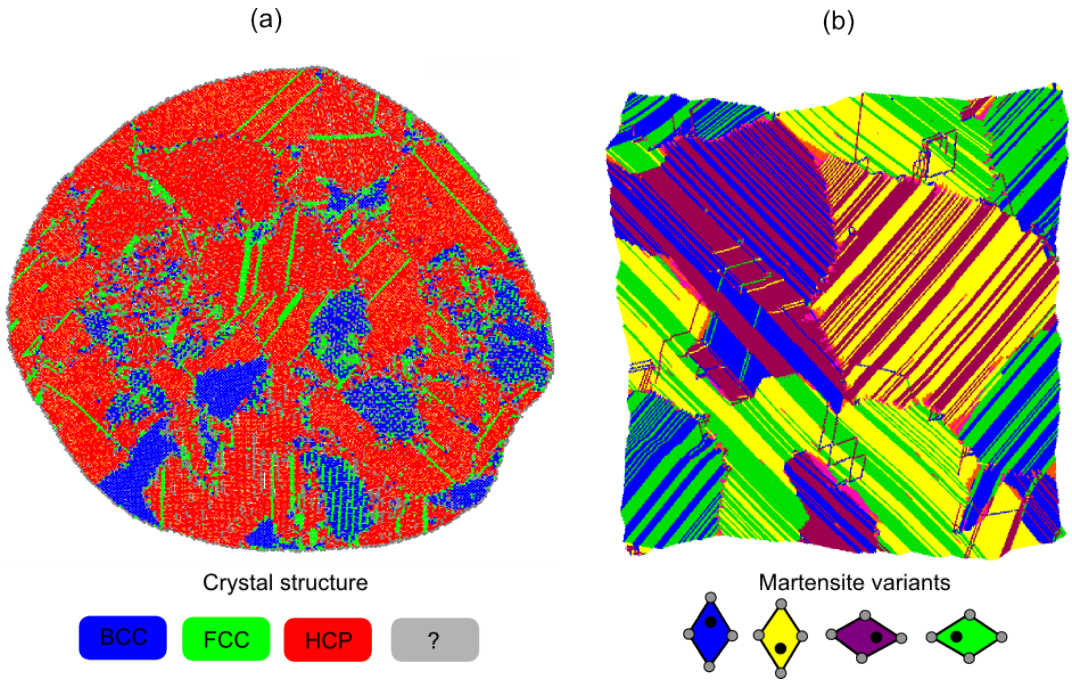
Shape memory alloys (SMA) exhibit a number of features which are not easily explained by equilibrium thermodynamics, including hysteresis in the phase transformation and "reverse" shape memory in the high symmetry phase. Processing can change these features: repeated cycling can "train" the reverse shape memory effect, while changing the amount of hysteresis and other functional properties. In the talk we present a molecular dynamics simulation study on this behaviour.

To simulate free evolutions of domain structures, atomic test assemblies must be sufficiently large and long computation times are required. Simulations of realistic 3D models therefore are limited by the computational ressources available. Therefore we employ a 2D Lennard-Jones model proven to represent a reliable qualitative model system for martensite/austenite transformations. We investigate the formation of microstructure and the evolution of defect structures in simulations of cyclic transformation/reverse transformation processes with this model. The simulations show that the transformation proceeds by non-diffusive nucleation and growth processes and produces distinct microstructure, see figure. Upon transformation, lattice defects are generated, which affect subsequent transformations and vary the potential energy landscape of the sample. If the sample is cycled through a series of forward/reverse transformations, the amount of defects in each phase accumulate. Defects act as nucleation sources for the transition. Moreover, the location of the defects can be preserved through the cycling, providing a memory of previous structures.



Molecular dynamics simulations of martensitic domain structure. (a): Zirconium, 3D, 3.5 Million atoms. (b): Lennard-Jones crystal, 2D, 160,000 atoms.