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The Role of Embedded Nanoclusters in Bcc-Iron in Hardening and Embrittlement of Reactor Pressure Vessel Steels as Revealed by Atomic Level Simulations

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The increase of computing power in recent years has made large scale simulation with million, or even billion of atoms is possible. Computer simulations using classical interatomic potentials are an efficient tool to study and understand materials properties and to investigate processes of materials on the atomic level. In this manner length and time scales can be considered which are often hardly accessible by experiments. In the talk two different applications of atomistic simulations are considered.

In the first topic the energetics and thermodynamics of the coherent copper nanoclusters in bcc-Fe are obtained using a combination of on-lattice Monte Carlo simulations and off-lattice molecular dynamics. These nanoclusters are assumed to be the main cause of hardening and embrittlement of Cu-bearing reactor pressure vessel steels since they act as obstacles to dislocation motion within the grains of the polycrystalline bcc-Fe.

The second topic about the fracture of ferrite steels (structural materials for nuclear fission reactors) during neutron irradiation in which the interaction between embedded nanocluster and an edge crack in the framework of linear elastic fracture mechanics (LEFM), are investigated at nanoscale using molecular static (MS) simulations.