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Title: Calibrating the Phase-Field Crystal Model for Grain Boundary Motion in Iron

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The Phase-Field Crystal (PFC) model provides a representation of the density as a continuous function, whose spatial distribution evolves in time at diffusional, rather than vibrational time scales. PFC provides a tool to study defect interactions at the atomistic level but over longer time scales than those achievable with MD. We examine the behavior of the PFC model with the goal of relating the PFC parameters to physical parameters of real systems, derived from MD simulations. For this purpose we model the phenomenon of the shrinking of a cylindrical or spherical grain situated in a matrix. The bi-crystal system in BCC is first created using the PFC model using parameters that stabilize the structure at the solidus temperature for pure iron. We then derive the positions of the atoms from the peaks of the Gaussion density profile and construct an atomistic model for MD. MD simulations are carried out using LAMMPS using a classical EAM potential. The PFC simulations are also continued to simulate the shrinking of the central grain driven by the free-energy gradient. By comparing the rates of shrinking of the central grain at different temperatures using MD and in PFC we derive the effective time step in PFC. It is shown that the relative speed-up between PFC and MD is problem specific. Research sponsored by Office of Basic Energy Sciences, DOE, through the Energy Frontier Research Center project, ?Center for Defect Physics.?