

From atomistic to mesoscale description of phase transitions

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Although the present understanding of atomic systems in thermodynamic equilibrium is rather satisfactory and is based on well established theoretical methods, the dynamic theory of atomic-scale evolution during phase transformation is far from completion in spite of extensive experimental and theoretical investigations. The highly nonlinear and nonequilibrium dynamics of phase transformations at mesoscale have been extensively studied by employing continuum Ginzburg-Landau-Khalatnikov (Phase Field) or Cahn-Hilliard-type kinetic equations. With random thermal noises, both types of equations become stochastic, and their applications to studying critical dynamics have been extensively discussed. During the past ten years, the phase-field approach has emerged as one of the most powerful method for modeling many types of microstructure evolution processes. However, it falls short in problems where crystalline defects have a profound influence on evolution in systems. Over the last few years, the phase field crystal (PFC) method has emerged as an attractive computational approach to tackle this class of problems where atomic and continuum scales are coupled. In the PFC method the higher order gradient terms has been added to the conventional isotropic Cahn-Hilliard equation. In this approach, the decomposition produces a periodical distribution of density clusters, which is attributed to a distribution of atoms in crystals. Imperfections in this periodical distribution well mimic lattice defects, dislocations and grain boundaries, while the decomposition mimics the crystallization. Despite of a significant progress in continuum description of atomic configurations using PFC method, the physical origin of the gradient terms in this model was not established. Recently, using Atomic Density Function (ADF) theory, this problem has been resolved by Jin and Khachatryan (JAP, 2006). It was shown that the choice of the gradient terms in PFC approach is equivalent to a smooth atom approximation. In this paper we show that the well known ADFs kinetic equations become automatically valid for the interacting atoms in the continuum when the lattice parameter of the underlying lattice is much smaller than the interaction radius, r_{int} . The relation between the ADF and Phase field approaches is under discussion.