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Pressure-Controlled Dynamic Equations of the PFC Model: A Mathematical Formulation

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Abstract : The phase-field-crystal, PFC, approach is a density-functional-type material model with an atomic resolution on a diffusive timescale. Spatially, the model incorporates periodic nature of crystal lattices and can naturally exhibit elasticity, plasticity and crystal defects such as grain boundaries and dislocations. Temporally, the model operates on a diffusive timescale which bypasses the need to resolve prohibitively small atomic-vibration time steps. The PFC model has been used to study many material phenomena such as grain growth, elastic and plastic deformations and solid-solid phase transformations. In this study, the pressure-controlled dynamic equation for the PFC model was developed to simulate a single-component system under externally applied pressure; these coupled equations are important for studies of deformable systems such as those under constant pressure. The formulation is based on the non-equilibrium thermodynamics and the thermodynamics of crystalline solids. To obtain the equations, the entropy variation around the equilibrium point was derived. Then the resulting driving forces and flux around the equilibrium were obtained and rewritten as conventional thermodynamic quantities. These dynamics equations are different from the recently-proposed equations; the equations in this study should provide more rigorous descriptions of the system dynamics under externally applied pressure.

Keywords : driving forces and flux, evolution equation, non equilibrium thermodynamics, Onsager’s reciprocal relation, phase field crystal model, thermodynamics of single-component solid
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