NUMERICAL STABILITY ANALYSIS OF PHASE-FIELD CRYSTAL MODELS

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The phase field crystal (PFC) model offers an effective continuum approach to numerically simulate crystallization processes on mesoscopic scales. Mathematically, this model is represented by a nonlinear parabolic differential equation involving sixth order spatial derivatives for the atomistic density as the phase field that locally minimizes an energy functional while preserving mass. The presence of sixth-order spatial derivatives combined with nonlinear equations present major difficulties for developing efficient numerical schemes that accurately captures the crystallization process and minimizes the energy with minimal numerical dissipation. In this work, we present a numerical scheme that is accurate, preserves mass and leads to energy dissipation with no numerical dissipation while effectively capturing the main physical features of the crystallization processes such as grain formation and defect evolution.

Keywords: Phase Field Crystal, Numerical Stability, Semi-Implicit Scheme, Finite Element Method, Nucleation and Growth