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An Energy Stable BDF2 Fourier Pseudo-Spectral Numerical Scheme for the Square Phase Field Crystal Equation

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Abstract. In this paper we propose and analyze an energy stable numerical scheme for the square phase field crystal (SPFC) equation, a gradient flow modeling crystal dynamics at the atomic scale in space but on diffusive scales in time. In particular, a modification of the free energy potential to the standard phase field crystal model leads to a composition of the 4-Laplacian and the regular Laplacian operators. To overcome the difficulties associated with this highly nonlinear operator, we design numerical algorithms based on the structures of the individual energy terms. A Fourier pseudo-spectral approximation is taken in space, in such a way that the energy structure is respected, and summation-by-parts formulae enable us to study the discrete energy stability for such a high-order spatial discretization. In the temporal approximation, a second order BDF stencil is applied, combined with an appropriate extrapolation for the concave diffusion term(s). A second order artificial Douglas-Dupont-type regularization term is added to ensure energy stability, and a careful analysis leads to the artificial linear diffusion coming at an order lower than that of surface diffusion term. Such a choice leads to reduced numerical dissipation. At a theoretical level, the unique solvability, energy stability are established, and an optimal rate convergence analysis is derived in the $\ell^\infty(0,T;\ell^2)\cap\ell^2(0,T;H_N^3)$ norm. In the numerical implementation, the preconditioned steepest descent (PSD) iteration is applied to solve for the composition of the highly nonlinear 4-Laplacian term and the standard Laplacian term, and a geometric convergence is assured for such an iteration. Finally, a few numerical experiments are presented, which confirm the robustness and accuracy of the proposed scheme.

AMS subject classifications: 35K30, 35K55, 65K10, 65M12, 65M70

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Key words: Square phase field crystal equation, Fourier pseudo-spectral approximation, second order BDF stencil, energy stability, optimal rate convergence analysis, preconditioned steepest descent iteration.

1 Introduction

The phase field crystal (PFC) model was proposed in [21] as a new approach to simulating crystal dynamics at the atomic scale in space but on diffusive scales in time. The model naturally incorporates elastic and plastic deformations, multiple crystal orientations and defects and has already been used to simulate a wide variety of microstructures, such as epitaxial thin film growth [22], grain growth [47], eutectic solidification [23], and dislocation formation and motion [47], to name a few. See the related review [41]. The key idea is that the phase variable describes a coarse-grained temporal average of the number density of atoms and the approach can be related to dynamic density functional theory [2,39]. This method represents a significant advantage over other atomistic methods, such as molecular dynamics methods where the time steps are constrained by atomic-vibration time scales. In more detail, the dimensionless energy is given by the following form [21,22,48]

$$E_{\rm pfc}(\phi)=\int_\Omega \left\{ \frac{1}{4}\phi^4+\frac{1-\varepsilon}{2}\phi^2-|\nabla\phi|^2+\frac{1}{2}(\Delta\phi)^2 \right\} d\mathbf{x}, \quad 0<\varepsilon, \tag{1.1}$$

where $\Omega\subset\mathbb{R}^D$, $D=2$ or 3, $\phi:\Omega\to\mathbb{R}$ is the atom density field. Typically the parameter ε which represents a deviation from the melting temperature, satisfies $0<\varepsilon<1$, though it may be possible that $\varepsilon>1$. In this paper, ϕ is assumed to be periodic on the rectangular domain Ω. Quite often, in the physics literature especially, the energy is rewritten as

$$E_{\rm pfc}(\phi)=\int_\Omega \left\{ \frac{1}{4}\phi^4-\frac{\varepsilon}{2}\phi^2+\frac{1}{2}\phi(1+\Delta)^2\phi \right\} d\mathbf{x}, \tag{1.2}$$

where

$$(1+\Delta)^2\phi=\left(1+2\Delta+\Delta^2\right)\phi=\phi+2\Delta\phi+\Delta^2\phi.$$

The two views of the energy allow us to analyze the convexity structure from different perspectives. In (1.1), we view the quadratic term $-|\nabla\phi|^2$ as destabilizing (concave), and $\frac{1-\varepsilon}{2}\phi^2$ (and all other terms) as stabilizing (convex). This view is valid only when $a:=1-\varepsilon$ is positive, which, as we have said, may be slightly restrictive. By contrast, in (1.2), we view $-\frac{\varepsilon}{2}\phi^2$ as destabilizing and all other terms as stabilizing. In either case, the phase field crystal (PFC) equation is defined as

$$\partial_t\phi=\Delta\mu, \quad \mu:=\delta_\phi E_{\rm pfc}=\phi^3-\varepsilon\phi+(1+\Delta)^2\phi.$$

When $\varepsilon<0$, the PFC equation can have solutions that exhibit spatial oscillations, and, typically in 2D, the peaks and valleys of ϕ are arranged in a hexagonal pattern. Such