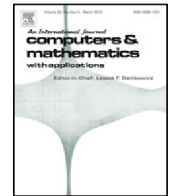




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# Convergence analysis and numerical implementation of a second order numerical scheme for the three-dimensional phase field crystal equation

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## ABSTRACT

In this paper we analyze and implement a second-order-in-time numerical scheme for the three-dimensional phase field crystal (PFC) equation. The numerical scheme was proposed in Hu et al. (2009), with the unique solvability and unconditional energy stability established. However, its convergence analysis remains open. We present a detailed convergence analysis in this article, in which the maximum norm estimate of the numerical solution over grid points plays an essential role. Moreover, we outline the detailed multigrid method to solve the highly nonlinear numerical scheme over a cubic domain, and various three-dimensional numerical results are presented, including the numerical convergence test, complexity test of the multigrid solver and the polycrystal growth simulation.

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## 1. Introduction

Defects, such as vacancies, grain boundaries, and dislocations, are observed in crystalline materials, and a precise and accurate understanding of their formation and evolution is of great interest. The phase field crystal (PFC) model was proposed in [1] as a new approach to simulate crystal dynamics at the atomic scale in space but on diffusive scales in time. This 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 [2], grain growth [3], eutectic solidification [4], and dislocation formation and motion [3,5]. The 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 [6,7]. The 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. More detailed descriptions are available in [3,8,9], and the related works for the amplitude expansion approach could be found in [8,10].

Consider the dimensionless energy of the form [1,2,11]:

$$E(\phi) = \int_{\Omega} \left[ \frac{1}{4}\phi^4 + \frac{1-\varepsilon}{2}\phi^2 - |\nabla\phi|^2 + \frac{1}{2}(\Delta\phi)^2 \right] dx, \quad (1.1)$$

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