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First- and second-order energy stable methods for the modified phase field crystal equation

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Abstract

The phase field crystal (PFC) model was extended to the modified phase field crystal (MPFC) model, which is a sixth-order nonlinear damped wave equation, to include not only diffusive dynamics but also elastic interactions. In this paper, we present temporally first- and second-order accurate methods for the MPFC equation, which are based on an appropriate splitting of the energy for the PFC equation. And we use the Fourier spectral method for the spatial discretization. The first- and second-order methods are shown analytically to be unconditionally stable with respect to the energy and pseudoenergy of the MPFC equation, respectively. Numerical experiments are presented demonstrating the accuracy and energy stability of the proposed methods.

Key words: Phase field crystal equation; Modified phase field crystal equation; Energy stability; Fourier spectral method

1 Introduction

Material properties are controlled by complex microstructures exhibiting topological defects, such as vacancies, grain boundaries, and dislocations. One of models for simulating these defects is the phase field crystal (PFC) equation proposed by Elder et al. [1,2]. The PFC equation is derived from a free energy

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