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Numerical Simulation of Phase-Field Round and Square Crystal Models on Curved Dynamic Substrates via the Evolving Surface Finite Element Method

Xufeng Xiao*, Lulu Liu, Xiao Yu and Xinlong Feng

College of Mathematics and System Sciences, Xinjiang University, Urumqi, Xinjiang 830046, China

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Abstract. This paper explores the formation of round and square crystals on curved dynamic substrates, employing the evolving surface phase field model as the mathematical framework and utilizing the evolving surface finite element method as the computational approach. The investigation focuses on the physical process of crystal growth on uneven, dynamic ultra-thin materials and biology thin films. The curved dynamic substrate is represented by the evolving surface. On evolving surfaces, two models, the classical phase field crystal model and the square phase field crystal model, are established and their respective physical properties are examined. Additionally, an efficient numerical simulation technique is devised by integrating the evolving surface finite element method with a time semi-implicit scheme. To validate the models, a series of numerical simulations are conducted to examine the physical properties and dynamical behaviors of the crystals formed under various conditions.

AMS subject classifications: 68W10, 74N05, 65M06

Key words: Phase-field crystal model, evolving surface finite element method, semi-implicit scheme, long time numerical simulation.

1 Introduction

The phase-field crystal (PFC) model serves as a continuum framework, grounded in density functional theory [1, 18, 32], designed to elucidate the microstructural evolution of crystalline materials. Through continuum approximation, this model seamlessly bridges atomic-scale microscopic details with macroscopic phase-field variables, facilitating precise simulations of crystalline microstructure dynamics. Its versatility renders it indispensable in materials science [14, 24, 32] for performance optimization, in the realm of

*Corresponding author.
Emails: xiaoxufeng111@sina.com (X. Xiao), liululumath@sina.com (L. Liu), yuxiaomath@yeah.net (X. Yu), fxlmath@xju.edu.cn (X. Feng)

physics [16, 37, 40] for exploring phase transitions and thermodynamic phenomena, and in engineering [19, 34, 36] for enhancing manufacturing processes.

The classical PFC equation, pioneered by Elder and his collaborators [12, 13], represents a seminal phase-field approach to modeling the dynamics of crystal growth. This sixth-order nonlinear evolution equation has found widespread application in investigating a diverse range of physical phenomena. Within this framework, one or more phase-field variables are introduced to delineate the spatial distribution of atomic density, enabling the simulation of intricate physical processes such as crystal growth, phase transitions, and the defect formation and evolution through the resolution of evolution equations for these phase-field variables [18, 40, 41]. As an important specialization of the PFC model, the square phase-field crystal (SPFC) model [4, 8, 38, 42] has emerged to address systems with square or analogous geometries. The SPFC model offers unparalleled precision in simulating and analyzing materials with square or geometrically similar configurations, thereby fostering a deeper comprehension of the intricate relationship between microstructure and material properties in these systems. The introduction of the SPFC model addresses the need for a tailored approach to handle the unique characteristics of such materials, distinguishing it from the more general PFC model and enriching the array of tools for materials research and development.

In recent years, the PFC model and the SPFC model have undergone substantial refinement and expansion. Efforts have been focused on enhancing their simulation accuracy, broadening their application scope, and integrating them with other multi-scale simulation techniques to enable cross-scale material simulations. When applying the equation in practical scenarios, upon obtaining its solution, we can obtain the concentration field, which represents the time-averaged coarse-grained atomic density. Previous literature has predominantly focused on the development and numerical analysis of the two models within static 2D and 3D frameworks, as documented in [9, 33, 39, 44]. Researches on the two models have been expanded to explore pattern formation on surfaces, as referenced in [25, 28]. The PFC model generates round phase crystals and the SPFC model generates square phase crystals. In 2D or 3D static regions, the above two models follow the mass conservation [43] and the energy dissipation law [35, 39].

Furthermore, the numerical simulations for the PFC model and the SPFC model can be adapted to accommodate evolving surfaces more broadly. The significance of studying the phase field crystal model on evolving surfaces lies in its ability to simulate and elucidate the dynamic processes and microstructural changes during material phase separation on the dynamic substrate, providing a powerful tool to comprehend the interplay between material properties and surface morphologies [21, 22]. Therefore, we aim to extend the PFC model and the SPFC model on evolving surfaces to expand their application scenarios. This paper formulates the PFC model and the SPFC model on evolving surfaces, offering an efficient numerical algorithm. In the process of mathematical modeling and the design of numerical algorithms, we want to satisfy the mass conservation and the energy dissipation law. However, we can only guarantee mass conservation at this stage. Regarding energy, further research is required. On an evolving surface, the veloc-