

The Stabilized Finite Element Method for the Cahn-Hilliard Phase-Field Model of Diblock Copolymers on Evolving Surfaces

Lulu Liu, Xufeng Xiao* and Xinlong Feng

*College of Mathematics and System Sciences, Xinjiang University,
Urumqi 830046, P.R. China*

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Abstract. This work focuses on the efficient numerical simulation of the Cahn-Hilliard phase-field model of diblock copolymers on evolving surfaces. The model integrates Cahn-Hilliard dynamic of diblock copolymers with partial differential equation on evolving surfaces, which has the property of geometric complexity, non-linearity and mass conservation. In the numerical simulation, the space-time discretization of the proposed model is realized by the evolving surface finite element method. The stabilized semi-implicit approach is included in the framework of the evolving surface finite element method to produce a linear, stable, conserved and high-accurate scheme for long time numerical simulations. The stability analysis of the designed numerical method is established. Through several numerical experiments, the convergence and stability of the numerical method are investigated. In addition, spinodal decomposition is performed to research the mass evolution and dynamics of the Cahn-Hilliard model of diblock copolymers on different evolving surfaces.

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Key words: Cahn-Hilliard model of diblock copolymers, evolving surface finite element method, stability analysis, long time numerical simulations.

1. Introduction

A diblock copolymer is a copolymer formed by the alternating arrangement of two different monomers repeatedly. It is widely used in nanotechnology [1, 2, 7], biomathematics [13, 25], film materials [30, 34], and other fields due to its many unique properties. The Cahn-Hilliard (CH) phase-field model of diblock copolymers is a mathematical model to describe the related evolution behaviors [3, 4, 23, 35]. It is based on the CH

*Corresponding author. *Email addresses:* liululumath@sina.com (L. Liu), xiaoxufeng111@sina.com (X. Xiao), fxlmath@xju.edu.cn (X. Feng)

equation with considering the concentration profiles of two different monomers on the copolymer chain. The idea of modeling is to introduce an order parameter to represent the difference between the concentration of the two categories of monomers. The evolution of the system can be viewed as the minimization of the total free energy functional in CH dynamics. The energy of the system is given by the nonlocal Ohta-Kawasaki functional which containing a nonlocal term that represents the first-order effects of the connectedness of the monomer chains [4, 6]. In [4, 24, 37], the authors have investigated the CH phase-field model of diblock copolymers, including the establishment of mathematical models, the design of reliable and effective numerical methods, and the numerical simulation in two- and three-dimensions.

The modeling of diblock copolymers on evolving domains is more general than that on two- and three-dimensional stationary domains. Therefore, it is interesting to investigate the dynamic behavior of this model on evolving surfaces, which corresponds to simulation studies on non flat and evolving substrates. This study is devoted to present the related mathematical modeling and numerical simulation approach. To explore the performance of the diblock copolymers on evolving surfaces, we construct the model by combining the CH dynamics of diblock copolymers and the partial differential equations on evolving surfaces. On the evolving surface, the developed model has the physical property of mass conservation. However, the velocity can be regarded as a force that is external, so the energy is not strictly dissipated. The property of energy is not studied in this paper, and more related content can be found in [19, 20].

To solve the CH model of diblock copolymers on the evolving surface, the related space-time discretization approaches should be reviewed. The evolving surface finite element method (ESFEM) [9–11, 27], stands as a widely-used space-time discretization technique that relies on a triangular mesh and variational formulation. Meshless methods are a class of methods that avoid mesh generation and have high accuracy. The common meshless approaches include the element-free Galerkin method [26, 31], the radial basis function finite differences (RBF-FD) method [22, 29], the moving least squares method [14, 15]. Although they avoid mesh generation, the numerical stability depends strongly on the distribution of surface nodes in the local stencil, and the related theoretical analyses are hard to be given. Taking into account both the operability of programming and the complexity of theoretical investigation, we select ESFEM as the fundamental method for space-time discretization in this study.

Another difficulty in designing the numerical method is avoiding the numerical instability caused by the small interface parameter for long time simulation. There are some mature and efficient numerical methods for settling models in 2D and 3D. Invariant energy quadratization (IEQ) [4, 24] and scalar auxiliary variable (SAV) methods [23] are widely used in the design of numerical algorithms. The fundamental idea behind these two approaches is to create a new equation that is of equal value to the original equation by bringing in suitable auxiliary variables and formulating the energy functional into a quadratic form. For the IEQ and SAV schemes, the numerical solution can only guarantee that the modified energy is monotonically nonincreasing, but it cannot obtain stability with respect to the original energy.