Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. **14**, No. 1, pp. 101-124

DOI: 10.4208/aamm.OA-2020-0293
February 2022

# A New Conservative Allen-Cahn Type Ohta-Kawaski Phase-Field Model for Diblock Copolymers and Its Numerical Approximations

Shuang Geng[1], Tongmao Li[1], Qiongwei Ye[2,*] and Xiaofeng Yang[3,*]

[1] *College of Management, Shenzhen University, Shenzhen, Guangdong 518060, China*
[2] *Business School, Yunnan University of Finance and Economics, Kunming, Yunnan 650221, China*
[3] *Department of Mathematics, University of South Carolina, Columbia, SC 29208, USA*

Received 15 September 2020; Accepted (in revised version) 8 January 2021

**Abstract.** We develop a new conservative Allen-Cahn phase-field model for diblock copolymers in this paper by using the Allen-Cahn type gradient flow approach for the classical Ohta-Kawaski free energy. The change in volume fraction of two composing monomers is eliminated by using a nonlocal Lagrange multiplier. Based on the recently developed stabilized Scalar Auxiliary Variable method, we have further developed an effective numerical scheme to solve the model. The scheme is highly efficient and only two linear and decoupled equations are needed to solve at every time step. We then prove that the numerical method is unconditionally energy stable, the stability and accuracy of the new scheme are demonstrated by numerous numerical examples conducted. By qualitatively comparing the equilibrium solution obtained by the new model and the classic Cahn-Hilliard model, we illustrate the effectiveness of the new model.

**AMS subject classifications**: 65N12, 65P40, 65Z05

**Key words**: Phase-field, Diblock copolymer, Allen-Cahn, nonlocal, second order, unconditional energy stability.

## 1 Introduction

The molecules of a block copolymer are composed of two or more segments of simple polymers (blocks). For instance, polymers of AB-type (called diblock) mean that every single chain is formed by a segment composed of the monomer A and a segment with monomer B. Recently, block copolymers have attracted great interest in the field

*Corresponding author.
*Emails:* gs@szu.edu.cn (S. Geng), litongmao@email.szu.edu.cn (T. Li), yqw@ynufe.edu.cn (Q. Ye), xfyang@math.sc.edu (X. Yang)

 

of science and engineering due to their highly adjustable self-assembly property in the nanoscale. That is, the copolymer system can self-assemble into various nanostructures, such as lamellar, cylinders, gyroids, and BCC (body-centered-cubic) phases, etc. To simulate the copolymer patterns and understand the process of formation of the copolymer chain, the diffusive interface phase-field method had been widely used as the effective modeling and simulation tool for this particular subject.

The basic idea of the phase-field method is to introduce a labeling function (phase-field variable) to represent the difference between the local volume fractions of the two constituent monomers, cf. [3, 5, 11, 16, 17, 22, 23]. For the diblock copolymer model, the total free energy usually consists of two parts, one of which is the linear part of gradient entropy, and the other is the nonlinear part containing the double-well potential and the so-called Ohta-Kawasaki nonlocal potential, see the pioneering work by Ohta and Kawaski in [17]. By using the variational method to minimize the assumed total free energy in the assumed metric, the governing PDE model can be further derived.

We note that the phase-field variable used in the diblock copolymer model is interpreted as the local volume fraction of the two monomers, so it is expected to conserve over time. Therefore, the model is generally derived using the Cahn-Hilliard dynamics ($H^{-1}$-gradient flow approach), thereby obtaining a fourth-order system. It is well-known that there is another gradient flow approach in phase-field modeling, the so-called Allen-Cahn dynamics ($L^2$-gradient flow approach). Note that the PDE system generated by the Allen-Cahn type model is second-order less than the PDE system of the Cahn-Hilliard model, which in turn brings weaker CFL conditions for grid size in time and/or space. Therefore, from a numerical point of view, the second-order Allen-Cahn model is preferable to the fourth-order Cahn-Hilliard model.

However, the Allen-Cahn model has an inherent defect that the volume cannot usually be conserved. To fix this issue, Rubinstein and Sternberg developed a so-called conservative Allen-Cahn equation, in which the variance of the total volume is offset by using a nonlocal Lagrange multiplier while retaining the law of energy dissipation. Inspired by this ingenious nonlocal technique, the first goal of this paper is to rebuild the diblock copolymer model using the lower-order Allen-Cahn dynamics. More precisely, after applying the variational method to the classic Ohta-Kawaski free energy in the $L^2$ space and adding a nonlocal Lagrange multiplier to offset the volume change, we arrive at a conservative nonlocal Allen-Cahn type PDE model for diblock copolymers. However, when designing a reliable and effective numerical algorithm for solving the new model, some new difficulties are encountered, especially how to discretize the newly added nonlocal term. In other words, if we directly apply the known methods that can successfully solve the local phase-field model, including simple-implicit [9], explicit [12, 13, 20, 27], convex-splitting [1, 8], etc., to deal with the newly obtained nonlocal model, the resulting numerical scheme will inevitably fail to maintain unconditional energy stability, or become a nonlinear scheme with actual high computational cost [15, 27].

Therefore, the second purpose of this article is to construct an effective numerical scheme to solve the new conservative Allen-Cahn diblock copolymer model. To this end,