

Ultraspherical Spectral Method for Block Copolymer Systems on Unit Disk

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Abstract. In this paper, we investigate ultraspherical spectral method for the Ohta-Kawasaki (OK) and Nakazawa-Ohta (NO) models in the disk domain, representing diblock and triblock copolymer systems, respectively. We employ ultraspherical spectral discretization for spatial variables in the disk domain and apply the second-order backward differentiation formula (BDF) method for temporal discretization. To our best knowledge, this is the first study to develop a numerical method for diblock and triblock copolymer systems with long-range interactions in disk domains. We show the energy stability of the numerical method in both semi-discrete and fully-discrete discretizations. In our numerical experiments, we verify the second-order temporal convergence rate and the energy stability of the proposed methods. Our numerical results show that the coarsening dynamics in diblock copolymers lead to bubble assemblies both inside and on the boundary of the disk. Additionally, in the triblock copolymer system, we observe several novel pattern formations, including single and double bubble assemblies in the unit disk. These findings are detailed through extensive numerical experiments.

AMS subject classifications: 65M70, 65M12

Key words: Block copolymer, Ohta-Kawasaki model, Nakazawa-Ohta model, disk domain, ultraspherical spectral method, bubble assembly, 'Head-to-tail' pattern.

1 Introduction

Block copolymers are macromolecules that contain monomers comprising different repeating units covalently linked together in polymer chains. Due to their remarkable ability for self-assembly, block copolymers form various nanoscale-ordered structures at thermodynamic equilibrium [1,2,4,19] and have attracted considerable theoretical and experimental interest over the past several decades [20,24,28,31]. Diblock copolymers,

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referred to as the binary system, comprise two distinct subchains made up of species A , and B , respectively. In contrast, triblock copolymers, known as the ternary system, consist of three subchains, each containing species A , B , and C , respectively.

In this paper, we begin with the Ohta-Kawasaki (OK) and Nakazawa-Ohta (NO) models introduced in [29, 31], which are general block copolymer systems with long-range interactions and describe the binary and ternary systems, respectively. In our study, we aim to explore the coarsening dynamic and pattern formations at equilibrium state in the OK/NO models in the disk domain.

Using the phase field labeling function $u = u(x)$ to represent the density of the species A and tracing the concentration of the species B by $1 - u(x)$, the OK model introduces the diblock copolymers by the following energy functional [58, 59]:

$$E^{\text{OK}}[u] = \int_{\Omega} \left[\frac{\epsilon}{2} |\nabla u|^2 + \frac{1}{\epsilon} W(u) \right] dx + \frac{\gamma}{2} \int_{\Omega} |(-\Delta)^{-\frac{1}{2}}(u - \omega)|^2 dx, \quad (1.1)$$

with a volume constraint

$$\int_{\Omega} u dx = \omega |\Omega|,$$

where $0 < \epsilon \ll 1$ is an interface parameter, $\Omega \subset \mathbb{R}^2$ is the spatial domain. $W(u) = 18(u^2 - u)^2$ is a double well potential which enforces the labeling function u to be 0 and 1 except the interfacial region between species A and B . The parameter γ represents the strength of the long-range repulsive interaction that favors the smaller size of the species and forces them to split in the OK model. Similarly, the free energy functional of the NO model [29] for the triblock copolymer system is defined as follows:

$$\begin{aligned} E^{\text{NO}}[u_1, u_2] = & \int_{\Omega} \frac{\epsilon}{2} (|\nabla u_1|^2 + |\nabla u_2|^2 + \nabla u_1 \cdot \nabla u_2) dx + \int_{\Omega} \frac{1}{\epsilon} W_2(u_1, u_2) dx \\ & + \sum_{i,j=1}^2 \frac{\gamma_{ij}}{2} \int_{\Omega} \left[(-\Delta)^{-\frac{1}{2}}(u_i - \omega_i) \times (-\Delta)^{-\frac{1}{2}}(u_j - \omega_j) \right] dx, \end{aligned} \quad (1.2)$$

where $u_i = u_i(x)$, $i = 1, 2$ are phase field labeling functions representing the density of species A and B , respectively. The concentration of species C can be implicitly described by $1 - u_1(x) - u_2(x)$. $W_2(u_1, u_2)$ is defined as

$$W_2(u_1, u_2) := \frac{1}{2} [W(u_1) + W(u_2) + W(1 - u_1 - u_2)],$$

and the volume constraints for u_1 and u_2 are

$$\int_{\Omega} u_i dx = \omega_i |\Omega|, \quad i = 1, 2.$$