Efficient and accurate numerical schemes for a hydro-dynamically coupled phase field diblock copolymer model

Qing Cheng, Xiaofeng Yang, Jie Shen

A1. Introduction

Block copolymer is a linear-chain molecule composed of two or more subchains linked together to create a polymer chain. When the subchain is made of two (or three) distinct monomer blocks, it is called diblock (or triblock) copolymer. Due to the incompatibility between the blocks, block copolymers undergo a micro-phase separation to form a periodic morphology in nanoscale, which provides an efficient technique to produce nano-structured materials and nano-devices (cf. [12,20,21,31,33,48]).

Modeling and numerical simulation are effective means to investigate the phase separation behaviors of block copolymer. In this paper, we consider the phase field based model for diblock copolymer (PF-BCP) model (cf. [4,7,8,16,26,32,48,50]) known as the dynamic mean field theory, where an order parameter is used to denote the difference between the local volume fractions of two monomers. The evolution of the PF-BCP system is derived from the energetic variation of the action function of the total free energy in the $H^{1}_{1}$ Sobolev space, i.e., the Cahn–Hilliard (CH) type equation. The total free energy for the system is the nonlocal Onsager–Kawasaki functional, that is the standard Cahn–Hilliard free energy supplemented with a nonlocal term, reflecting the first order effects of the connectivity of the monomer chains (cf. [7,32]). Due to its complexity, particularly the inclusion of a nonlocal potential, it is challenging to develop accurate, stable and efficient numerical