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Short Polymer Modeling using Self-Consistent Integral Equation Method[1] YEONGYOON KIM, SO JUNG PARK, JAEUP KIM, UNIST — Self-consistent field theory (SCFT) is an excellent mean field theoretical tool for predicting the morphologies of polymer based materials. In the standard SCFT, the polymer is modeled as a Gaussian chain which is suitable for a polymer of high molecular weight, but not necessarily for a polymer of low molecular weight. In order to overcome this limitation, Matsen and coworkers have recently developed SCFT of discrete polymer chains in which one polymer is modeled as finite number of beads joined by freely jointed bonds of fixed length. In their model, the diffusion equation of the canonical SCFT is replaced by an iterative integral equation, and the full spectral method is used for the production of the phase diagram of short block copolymers. In this study, for the finite length chain problem, we apply pseudospectral method which is the most efficient numerical scheme to solve the iterative integral equation. We use this new numerical method to investigate two different types of polymer bonds: spring-beads model and freely-jointed chain model. By comparing these results with those of the Gaussian chain model, the influences on the morphologies of diblock copolymer melts due to the chain length and the type of bonds are examined.

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