

Abstract Submitted
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Computational Models of Complex Microstructures of Amphiphilic Diblock Copolymers in Dilute Solution¹ JESSE BOER, APICHART LINHANANTA, Department of Physics, Lakehead University — The formation of micelles and vesicles in dilute solutions of amphiphilic diblock copolymers are investigated by the real-space self-consistent field theory (SCFT) in two dimensions and by a Monte-Carlo lattice model in three dimensions. The real-space SCFT method produced rodlike and spherulike micelles and vesicles. It is found that the shapes of the microstructures are determined by the initial conditions in the SCFT algorithms, and that, in general, vesicles have lower free energy than micelles. In contrast, in the Monte Carlo simulation of the lattice model, it is found that as the volume fraction of copolymer increases, the microstructure go from spherulike micelles to rodlike micelles to vesicles and, at high fraction, to the lamellar phase.

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