

Fluctuations/Correlations in Symmetric Diblock Copolymers: Direct Comparisons Between Simulations and Theories

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Here we unambiguously quantify the fluctuation/correlation effects by direct comparisons between the newly proposed fast off-lattice Monte Carlo (FOMC) simulations¹ and the corresponding theories based on exactly the same model system (Hamiltonian), thus without any parameter-fitting. The symmetric diblock copolymers are modeled as discrete Gaussian chains with soft, finite-range repulsions as commonly used in dissipative-particle dynamics simulations. The effects of chain discretization and finite-range interactions on the order-disorder transition (ODT) are properly accounted for in our mean-field theory.² Our FOMC simulations are performed in a canonical ensemble with variable box lengths to eliminate the adverse effects of fixed box.³ The thermodynamic and structural properties of both the disordered and lamellar phases are studied in the simulations. Furthermore, with a new order parameter for the lamellar phase, we use replica exchange and multiple histogram reweighting to accurately locate ODT in our simulations. Our FOMC results for the disordered phase are further compared, without any parameter-fitting, to those from the reference interaction site model (RISM) and the polymer reference interaction site model (PRISM) theories, as well as the Gaussian fluctuation theory, based on the same model system. Such direct comparisons unambiguously and quantitatively reveal the consequences of various theoretical approximations and the validity of these theories in describing the fluctuations/correlations in disordered diblock copolymers.

[1] Q. Wang and Y. Yin, *J. Chem. Phys.*, **130**, 104903 (2009).

[2] Q. Wang, *J. Chem. Phys.*, **129**, 054904 (2008); **131**, 234903 (2009).

[3] Q. Wang, *J. Chem. Phys.*, **129**, 054904 (2008); **131**, 234903 (2009).