Symmetric Diblock Copolymers in Nanopores: Monte Carlo Simulations and Strong-Stretching Theory

QIANG WANG, Colorado State University — We have performed lattice Monte Carlo simulations to study the self-assembled morphology of symmetric diblock copolymers in nanopores. The pore diameter and surface preference are systematically varied to examine their effects on the chain conformations, structures of various morphologies and their phase transition. Various ensemble-averaged profiles and quantities are used to provide detailed information about the system. The simulation results are also compared with the predictions of a strong-stretching theory commonly used in the literature. Such comparisons reveal the deficiencies of this theory in describing the morphologies under cylindrical confinement, and call for further theoretical studies using more accurate formalisms.

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