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Brownian Dynamics Simulation of ABA Block Copolymer in Selective Solvent: Kinetics of HEX Cylinders to BCC Spheres Transition[1]
MINGHAI LI, YONGSHENG LIU, RAMA BANSIL, Boston University — A Brownian Dynamics simulation was performed on 200 bead spring chains of triblock copolymer, $A_{10}B_{10}A_{10}$. The repulsive interactions of A monomers (in good solvent) are modeled by the Weeks-Chandler-Anderson potential. The poor solvent attraction of the B monomers is described by a Lennard-Jones (LJ) potential. We have determined the phase diagram of 30% ABA block copolymer in a selective solvent for the A block. At temperature T=1 (in units of ε/k_B, where ε is the well depth of the LJ interaction potential and k_B the Boltzmann constant) the equilibrium state is HEX cylinder; at T=1.5 the system is in BCC spheres. We follow the time evolution of the HEX to BCC transition by jumping from T=1 to 1.5. The Fourier transform is calculated at each time-step in the simulation and compared to time-resolved small angle x-ray scattering data from triblock copolymer solution (Kraton G1650 in mineral oil). The simulation is also compared with a calculation based on a geometric model of coupled anisotropic fluctuations to describe the transition from HEX cylinders to BCC spheres.

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