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Brownian Dynamics Simulation of Kinetics of HEX Cylinders to FCC Spheres Transition in ABA Triblock Copolymer in Selective Solvent[1]

MINGHAI LI, Boston University, RAMA BANSIL[2], Boston University and National Science Foundation — We report Brownian Dynamics simulations on 400 bead-spring chains of triblock copolymer, $A_{10}B_{10}A_{10}$, in a selective solvent for the A block using a FENE potential together with Lennard-Jones (LJ) for B-B attraction and a Weeks-Chandler-Anderson potential for A-B and A-A repulsions. On varying volume fraction and temperature T (in units of ε/k_B, where ε is the well depth of the LJ interaction and k_B the Boltzmann constant) we observe spheres in cubic phases, HEX cylinders, worm-like and disordered micelles. The time evolution following a quench from T= 0.8 to 0.5 shows a nucleation and growth mechanism where one cylinder breaks into spheres and induces neighboring cylinders to break into spheres. This observation is confirmed by calculating the density profile of each cylinder and Fourier transform of the density distribution. We also performed jumps at constant T = 0.8 by changing the LJ well depth (ε) from 1 to various higher values. We found that for $\varepsilon > 4$ the cylinders are kinetically trapped, and the transition is fastest for $\varepsilon = 1.5$.

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