

Kinetics of Order-order transitions in block copolymers: Cylinders to spheres

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Summary

Block copolymers are known to form micelles of different shapes in selective solvents that preferentially dissolve one of the constituent blocks. These micellar fluids exhibit various ordered and disordered phases. To gain microscopic insight into the mechanisms involved in the transformation between different phases we use synchrotron-based time-resolved small angle x-ray scattering (SAXS) and coarse-grained discrete Brownian Dynamics simulations. In this talk I will focus on the kinetics of the transformation from the hexagonal packed cylinder (HEX) phase to cubic phases (FCC or BCC). SAXS data was interpreted with a geometrical model for the transformation from cylinders to spheres. Brownian Dynamics simulation for an ABA triblock copolymer in a solvent selective for the A block will also be presented. In this system isolated micelles containing B in the core and A in corona are formed. The kinetics of the transformation was investigated by following the time evolution of the simulated system following an instantaneous jump in temperature or by changing the depth of the Lennard-Jones potential well. Detailed analysis showed that the transformation occurred via a rippling mechanism, with the ripple starting on one cylinder and then inducing ripples in neighboring cylinders. The real space morphological data obtained in the simulation was Fourier transformed to obtain the structure factor measured in scattering experiments, so as to directly compare simulation with SAXS data. The results indicated that the order-order transformation was a nucleation and growth process when the temperature of the system instantly jumped from 0.8 to 0.5.

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