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Cubic Micellar Crystals of $A_nB_mA_n$ Block Copolymers from MD[1]
CHRIS LORENZ, Kings College London, JOSHUA ANDERSON, ALEX TRAVESSET, Iowa State University and Ames Laboratory — Amphiphilic block copolymers exhibit a wide variety of phases in solution. One common phase of $A_nB_mA_n$ polymers is made up of spherical micelles with hydrophobic (B) cores and hydrophilic (A) coronas. At high enough concentrations, these micelles order on a lattice forming a micellar crystal. The dynamics during the formation of this phase are fascinating, being controlled almost entirely by the polymer transfer between micelles, as shown in Molecular Dynamics simulations. Application of a standard nucleation and growth analysis shows that the micellar crystals grow extremely rapidly and are probably aided by the periodic box in the simulation. A study of the dynamics at equilibrium shows that polymer transfer is still a continuing process and can be understood in the context of transition state theory.

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