

Morphology and conformation analysis of self-assembled triblock copolymer melts.

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Abstract

We used the dissipative particle dynamics method to simulate the self-assembly of sym. triblock copolymers of the type ABA. Depending on the vol. fraction of the end blocks f_A , several mesophases including lamellar, perforated lamellar, gyroid, hexagonal cylinders and bcc spherical micelles were obtained. The order-disorder transition (ODT) at $f_A = 0.5$ was found to be about $\chi N = 19.8$. The ODT for the cylindrical mesophase at sym. points on the phase diagram had different values, indicating asymmetry in the phase diagram. We were also able to est. the bridge fraction in the different mesophases. They range from about 0.44 for the lamellar mesophase to about 0.75 for the spherical micelles. Our simulation results are in good agreement with previously reported theor. calcns. and exptl. observations.