Mixed Lamellae in Symmetric Diblock Copolymer Thin Films

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For symmetric diblock copolymers confined between two flat and homogeneous surfaces, three morphologies (parallel, perpendicular, and mixed lamellae) have been obtained in experiments. The effects of surface preference (for one of the two blocks) and film thickness on the thin-film morphology are well understood. Less studied is the copolymer chain conformation near a hard (impenetrable) surface, referred to as the "hard-surface effect". It is this effect that favors the formation of perpendicular lamellae between two neutral surfaces over parallel lamellae at all film thicknesses. It also leads to the possible formation of mixed lamellae between asymmetric surfaces (not antisymmetric ones, where the two surfaces prefer different blocks with the same strength).

In this work, we use the self-consistent field theory in continuing to study the morphology of mixed lamellae in both 2D and 3D. A parallel algorithm is used to solve the SCF equations in real space with high accuracy. Results under different boundary conditions (zero-density vs. non-flux) are compared in order to examine their influence on the copolymer chain conformation near the surface, and on the free energy of mixed lamellae. We also study, in detail, the chain conformation at the T-junction in this morphology. The conditions under which the mixed lamellae are in a stable phase are determined quantitatively. We finally compare our SCF calculations with available experimental and simulation results.