

## Dynamics of Single-Chain Conformations in Triblock Copolymers

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In the lamellar phase of symmetric ABA triblock copolymers, the middle block B can either form a loop or a bridge. A loop consists of a B block whose two ends are located on the same internal AB interface. A bridge straddles a B domain. Since converting loops into bridges or vice versa requires an A block to move across a B domain, it involves a large free-energy barrier for the single-chain dynamics. Thus, the relaxation of loops and bridges in a segregated lamellar phase is intrinsically slow and a configuration is not only characterized by the composition profile but, additionally, by a slow variable that characterizes the chain conformations. We choose to describe the nonequilibrium chain conformations by the variance of the first Rouse mode  $X_1^2$ , and demonstrate that there is a strong correlation between  $X_1^2$  and the fraction of loops. Using self-consistent field theory (SCFT) we calculate the free-energy of a lamellar phase with a fixed value of  $X_1^2$  and derive a dynamic SCFT including the corresponding Onsager coefficient for the disordered and the lamellar phase. We argue that the system can be mapped onto a set of independent two-state Markov models and extract the transition rates from short simulation runs, using a soft, coarse-grained particle model. This strategy allows us to estimate the relaxation of the loop fraction and its equilibrium value and speed up the simulation via a heterogeneous multiscale method.