Protracted Colored Noise Dynamics Applied to Molecular Dynamics Simulations of Block Copolymers

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Mean field models and Monte Carlo simulations have been used to study polymeric systems in recent years. While these methods provide great computational expedience, they include less accurate potentials and require intelligently selected modes of motion, which can adversely affect outcomes. Conversely, molecular dynamics (which uses Newton's second law to calculate molecular movements) combined with realistic potentials provide more accurate movements and states, though computational efficiency is sacrificed. Using coarse graining and parallel computing greatly increases the time and length scales that can be accessed in MD simulations of polymeric systems, but some systems, especially systems with large energy barriers or with long chains, still require unrealistic simulation times. One example of such a system is a lamellar forming BCP with a defect. Although the defect density is very small at equilibrium, the activation energy can be large, causing a drastic increase in computation time.

The purpose of this study is to apply protracted colored noise dynamics (PCND) to such systems with the goal of decreasing the simulation time required to reach equilibrium. PCND is a technique that applies time correlated stochastic forces in MD simulations. In linear polymer systems these forces can be made to act along the backbone of the chain. These forces broaden the energy distribution of the system, increasing the diffusivity of the molecules, and allowing energy barriers to be passed over more easily. Of course, the distribution of these forces must be carefully chosen so that the equilibrium state is not excessively perturbed. In this study, PCND was applied to BCP simulations from two initial states: mixed state, and defective lamellar state. The results of the mixed state simulations were used to fine tune PCND parameters to avoid excessive perturbation of system behavior. The defective state simulations were used to determine how much PCND would reduce computational time. The results have been promising, showing an order of magnitude reduction in computational time required to reach equilibrium for defective state simulations.