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Monte Carlo simulations of a coarse-grain model for block-copolymer melts: method and application FRANCOIS DETCHEVERRY, DARIN PIKE, PAUL NEALEY, JUAN DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin - Madison, Madison, WI 53706, MARCUS MUELLER, Institut fur Theoretische Physik, Georg-August Universitat, 37077 Goettingen, Germany — A new Monte Carlo based approach has been developed for simulation of polymeric systems, including block copolymers. The approach represents the system at the level of a coarse-grain Hamiltonian, akin to that employed in widely used self-consistent field theoretic (SCFT) treatments. In contrast to traditional implementations of SCFT, however, molecules are treated explicitly and fluctuations are taken into account. We present two distinct implementations of the method; the first relies on a grid, and the second does not. While the grid-based method is highly computationally efficient, the gridless implementation permits simulations in arbitrary ensembles, including the grand-canonical and Gibbs ensembles, thereby facilitating study of phase transitions. The gridless implementation also gives access to the local mechanical properties. The performance of the two implementations is discussed in the context of several applications, including the directed assembly of multi-block copolymer thin films on patterned substrates, either chemical or topographical. In both cases we examine the ordering of the material and the effect of pattern or surface roughness.

Francois Detcheverry
member

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