Bulk and interfacial thermodynamics of a symmetric, ternary homopolymer-copolymer mixture: a Monte Carlo study

M. Müller and M. Schick
Department of Physics, Box 351560 , University of Washington
Seattle, Washington 98195-1560
(October 6, 1997)

We present results of a Monte Carlo simulation of a dense blend, comprising two incompatible homopolymers and a symmetric diblock copolymer, all of the same degree of polymerization. The simulations, in the framework of the bond fluctuation model, yield information on the phase diagram. At high temperatures the copolymer dilutes the homopolymer blend and shifts the critical temperatures of the unmixing transition to lower temperatures. The line of second order transitions ends in a tricritical point, below which there is three-phase coexistence between two homopolymer-rich phases and a spatially-structured copolymer-rich one. The simulations indicate that this latter phase is a microemulsion at intermediate incompatibility, and a lamellar phase at high incompatibility. Using a multimagnetic reweighting scheme, we determine independently the reduction of the interfacial tension and the copolymer excess at the interface between the coexisting homopolymer-rich phases. The bending rigidity is estimated by measuring the spectrum of interfacial fluctuations. We outline a method to determine the interaction between copolymer monolayers, and find that in the two-phase region, it is attractive and its range increases upon addition of copolymers.