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Gibbs Ensemble Calculations of Phase Coexistence in Supramolecular Assembly of Block Copolymers ZOLTAN MESTER, NATHANIEL LYND, GLENN FREDRICKSON, University of California Santa Barbara — We propose a new self-consistent field theory method for calculating phase behavior in reversibly bonded supramolecular polymer melts. Previous studies formulated models for supramolecular assembly in the grand canonical ensemble to make use of the constraints imposed on the chemical potentials of the products from chemical equilibrium. Instead, we formulate the model in the canonical ensemble by including a term in the Hamiltonian that accounts for the reaction favorability/penalty. The chemical equilibrium statement is obtained by optimizing the Hamiltonian with the amount of reacted polymer. The canonical partition function can be easily adapted to the Gibbs ensemble whereby phase boundaries between coexisting phases can be conveniently simulated. As an illustration of our method, we examine a blend of AB diblock and B homopolymer with the ability to reversibly bond to form ABB diblock. In the limits of infinite reaction favorability and penalty, the system approaches cases of an ABB diblock-B homopolymer blend when the AB diblock is the limiting reactant and an AB diblock-B homopolymer blend, respectively. The interplay between reactant ratios (stoichiometry) and reaction favorability/penalty is explored for intermediate values of reactivity.

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