Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Phase coexistence calculations via a unit-cell Gibbs ensemble formalism for melts of reversibly bonded block copolymers ZOLTAN MESTER, NATHANIEL LYND, GLENN FREDRICKSON, University of California, Santa Barbara — Melts of block copolymer blends can exhibit coexistence between compositionally and morphologically distinct phases. We derived a unit-cell approach for a field theoretic Gibbs ensemble formalism to rapidly map out such coexistence regions. We also developed a canonical ensemble model for the reversible reaction of supramolecular polymers and integrated it into the Gibbs ensemble scheme. This creates a faster method for generating phase diagrams in complex supramolecular systems than the usual grand canonical ensemble method and allows us to specify the system in experimentally accessible volume fractions rather than chemical potentials. The integrated approach is used to calculate phase diagrams for AB diblock copolymers reversibly reacting with B homopolymers to form a new diblocks we term "ABB." For our case, we use a diblock that is sixty percent A monomer and a homopolymer that is the same length as the diblock. In the limits of infinite reaction favorability (large equilibrium constant), the system approaches cases of an ABB diblock-B homopolymer blend when the AB diblock is the limiting reactant and AB diblock-ABB diblock blend when the homopolymer is the limiting reactant. As reaction favorability is decreased, the phase boundaries shift towards higher homopolymer compositions so that sufficient reaction can take place to produce the ABB diblock that has a deciding role stabilizing the observed phases.

Zoltan Mester
University of California, Santa Barbara

Date submitted: 26 Nov 2012 Electronic form version 1.4