Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Identification of self consistent field interaction parameter from continuum Monte Carlo simulation of model polymer blends JUN KYUNG CHUNG, DAVID MORSE, University of Minnesota — Monte Carlo simulations of binary AB polymer blends have been performed to evaluate the effective interaction parameter χ_e of self consistent field theory, and to quantify corrections to RPA predictions for fluctuations. We consider a model with a non-bonded pair interaction $v_{ij}(r) = \epsilon_{ij} f(r)$ for which $f(r)$ is of the repulsive Lennard-Jones form, $\epsilon_{AA} = \epsilon_{BB}$, and $\epsilon_{AB} = \epsilon_{AA} + \Delta\epsilon$. Using thermodynamic perturbation theory, to first order in $\Delta\epsilon$, we obtain an interaction free energy with the composition dependence predicted by Flory-Huggins theory, with an effective interaction parameter $\chi_e = \Delta\epsilon z_c$. Here, z_c is an effective coordination number given by the average of the sum of values of $f(r)$ for interactions between a test monomer and nearby monomers on other chains, in a reference system with $\Delta\epsilon = 0$. Results for composition fluctuations in semigrand ensemble simulations of blends with a range of values of $\Delta\epsilon \neq 0$, for several chain lengths, are compared to RPA predictions calculated using this perturbatively defined χ_e parameter.

Jun Kyung Chung
University of Minnesota

Date submitted: 27 Nov 2007 Electronic form version 1.4