Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Multi-scale simulation of dynamical properties of polymer blend interfaces BHARADWAJ NARAYANAN, VICTOR PRYAMITSYN, VENKAT GANESAN, The University of Texas at Austin — We present the results of a multiscale simulation approach which combines Brownian dynamics simulations with polymer self- consistent field theory and continuum mechanics to study two effects: (i) The dynamical properties of polymer blend interfaces and the influence of block copolymer compatiblizers; (ii) The effect of externally applied simple shear flow on the phase behavior of polymer blends. In the first context, our numerical results agree quite well with the predictions from scaling approaches and phenomenological theories. Moreover, these results also provide a microscopic explanation of the negatively deviating viscosities of polymer blends. We also present results elucidating the "slip suppressing" influence of block compatiblizers. In the second context, we explore the effects of visoelastic asymmetry and the composition dependence of polymer mobilities as driving forces for shear induced mixing and de-mixing phenomena seen in polymer blends. Our results suggest a rich variety of behavior arising from the interplay between viscoelasticity and thermodynamics and is in qualitative agreement with other theories and experimental observations.

Bharadwaj Narayanan
The University of Texas at Austin

Date submitted: 02 Dec 2004 Electronic form version 1.4