Abstract Submitted for the MAR05 Meeting of The American Physical Society

Capillary Waves, Chain Conformations, and Viscoelasticity at Sheared Blend Interfaces: DSCF - MD Comparison. TAK LO, MAJA MI-HALJOVIC, YITZHAK SHNDIMAN, Dept of Physics, College of Staten Island, CUNY, WENTAO LI, DILIP GERSAPPE, Dept of Materials Science and Engg, SUNY at Stony Brook NY 11794 — We have recently improved a previously proposed dynamic self-consistent field (DSCF) lattice theory of polymer fluids by accounting for transient viscoelastic effects in time evolution. We have applied the DSCF theory to study both the time evolution and the steady state chain conformation and rheology at interfaces of sheared, immiscible polymer blends. While DSCF allows direct determination of interfacial morphology and rheology evolution, chain conformation statistics was sampled with a Monte Carlo process using the probability distributions and transition rates generated by the DSCF equations. The results were compared to molecular dynamics (MD) simulations. We found that discrepancy with MD results is minimized if broadening of the DSCF interface by capillary wave fluctuations is accounted for.

> Dilip Gersappe Dept of MSE, SUNY at Stony Brook

Date submitted: 01 Dec 2004

Electronic form version 1.4