Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Coarse grained model of polymer dynamics R.C. PICU, A. RAKSHIT, Rensselaer Polytechnic Institute — A coarse grained representation of the structure and dynamics of polymer melts is developed. In the coarse grained model an entanglement segment is represented as a blob with a single degree of freedom. The inner blobs of the chain are constrained to perform random walks along the primitive path, while the chain end blobs have three degrees of freedom and interact through a non-bonded potential with all other blobs of the system. The primitive path is initially calibrated from the fine, atomistic system and then evolves as dictated by the kinematics of the end blobs. The inter-blob bonded and non-bonded potentials are calibrated from the fine model to reproduce the chain structure statistics. The coarse system is evolved with Brownian dynamics using a monomeric friction which is computed from the fine system. Constraint release is introduced and is dictated by an error indicator that monitors the neighborhood of a given primitive path segment during the simulation. The only parameter which is not necessarily (but it may be) calibrated from the fine model is the characteristic entanglement segment length. The coarse model predictions are compared with full atomistic simulation results.

R.C. Picu
Rensselaer Polytechnic Institute

Date submitted: 19 Nov 2006 Electronic form version 1.4