Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Molecular dynamics studies of slow relaxation phenomena in glassy polymeric systems. SANAT KUMAR, SERGEI SHENOGIN, Rensselaer Polytechnic Institute, ARUN YETHIRAJ, University of Wisconsin, Madison, JACK F. DOUGLAS, Polymer Division, NIST, Gaithersburg, MD. — Molecular dynamics simulations were used to study long-time structural relaxations in glass-forming polymeric systems. The model system was composed of identical hard spherical beads linked into the chains by the bonds. The minimum length of each bond was limited to 1.05 of the bead diameter to prohibit crystallization at higher densities and create completely amorphous structures. The packing volume fraction ranges from 0.45 to 0.62, with glass transition at volume fraction around 0.565. It was shown that for glassy structures the distribution of mean-squared displacements deviates from Fickian form, showing the presence of "mobile" particles with caged (hop-like) mechanism of mobility. As the result, dynamic heterogeneity emerges in glassy structures with two distinct distributions of "mobile" and "immobile" particles relative to the Brownian motion. Structural relaxation, shear viscosity and their relationship to particle mobility was studied for systems with different densities. These results provide the evidence that the excessive mobility of "hopping" particles is the reason of breakdown of Stokes-Einstein relationship in glassy systems.

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Date submitted: 11 Jan 2006

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