Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Molecular simulation investigation of the nanorheology of an entangled polymer melt MIR KARIM, RAJESH KHARE, Texas Tech Univ, TSUTOMU INDEI, JAY SCHIEBER, Illinois Institute of Technology — Knowledge of the "local rheology" is important for viscoelastic systems that contain significant structural and dynamic heterogeneities, such as cellular and extra-cellular crowded environments. For homogeneous viscoelastic media, a study of probe particle motion provides information on the microstructural evolution of the medium in response to the probe particle motion. Over the last two decades, probe particle rheology has emerged as a leading experimental technique for capturing local rheology of complex fluids. In recent work [*M. Karim, S. C. Kohale, T. Indei, J. D. Schieber, and R. Khare, Phys. Rev. E* ***86****, 051501 (2012)*], we showed that this approach can be used in molecular dynamics (MD) simulations to study the nanoscale viscoelastic properties of an unentangled polymer melt; an important conclusion of that work was that medium and particle inertia play a crucial role in analysis of the particle rheology simulation data. MD simulations have a natural advantage that they enable study of deformation and dynamics over a small length scale around the moving probe particle. In this work, the approach is extended to compare the motion of a nanoscale probe in melts of entangled and unentangled chains. The simulations will be used to elucidate the differences between the local responses of these media to the probe particle motion. In particular, results will be presented for the differences in the resultant velocity and stress fields as well as any possible structural asymmetry developed around the moving probe particle in the entangled and unentangled cases.

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Date submitted: 15 Nov 2013 Electronic form version 1.4