Abstract Submitted
for the PSF13 Meeting of
The American Physical Society

Supported shock waves in hydroxyl-terminated polybutadiene melts: A large-scale molecular dynamics study MARKUS FROEHLICH, THOMAS SEWELL, DONALD THOMPSON, University of Missouri-Columbia — Hydroxyl-terminated polybutadiene (HTPB) melts subjected to supported shock loading were studied by non-reactive all-atom molecular dynamics (MD) simulations to investigate their responses to shock wave passage. An efficient Monte Carlo/MD technique was developed to generate multi-million-atom systems of well-equilibrated linear polymers with chain lengths $n = 64$, 128, or 256 backbone carbons. Explicit shock wave simulations, performed using a reverse-ballistic method, were carried out for all three chain lengths with a shock strength of 8.6 GPa, and for the $n = 128$ system with four different shock strengths ranging from 2.8 to 12.5 GPa. All MD simulations were done using LAMMPS and the OPLS-AA force field with the Lennard-Jones potential replaced by the Buckingham exp-6 potential. Spatial and temporal resolution of the shock response was obtained by analyzing the simulation data in a reference frame centered on the shock front, which traverses the sample with constant speed. Structural properties, global scaling behaviors, and vibrational spectra of the unshocked polymers are in good agreement with literature data. Results for the shocked material indicate a shock-induced transition to a glass-like state based on residual shear stresses and increases of structural relaxation times by several orders of magnitude. Vibrational spectra for the shocked states exhibit considerable broadening and blue shifting.

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Date submitted: 10 Oct 2013 Electronic form version 1.4