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Molecular dynamics study of the shock response in hydroxyl-terminated polybutadiene melts[1] MARKUS G. FROEHLICH, THOMAS D. SEWELL, DONALD L. THOMPSON, Department of Chemistry, University of Missouri-Columbia — All-atom molecular dynamics (MD) simulations using the non-reactive OPLS-AA force field were performed to study the detailed structural, mechanical, and spectroscopic response of hydroxyl-terminated polybutadiene (HTPB) melts subjected to supported shock waves. A combination of Monte Carlo and MD techniques was used to generate thoroughly equilibrated initial configurations, for monodisperse systems with chain lengths ranging from 64 to 256 backbone carbons per chain. Properties characterizing the size, shape and orientation of single chains, as well as the vibrational density of states, were evaluated prior to and following shock passage for four impact velocities between 1.0 and 2.5 km/s. The structural properties and global scaling behaviors of the unshocked systems are in excellent agreement with literature data. Results for the shocked systems, obtained using a geometric binning approach that provides spatio-temporal resolution in the reference frame centered on the shock front, indicate a transition to a glass-like state with a concomitant increase by several orders of magnitude of structural relaxation times in the shocked material.

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