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A Molecular Dynamics Simulation Study of the Alpha- and Beta-Relaxation Processes in a Realistic Model Polymer DMITRY BEDROV, GRANT D. SMITH, University of Utah — Molecular dynamics simulations of a melt of freely rotating chains of 1,4-polybutadiene (FRC-PBD) have been performed over a wide range of temperature. Removal of the dihedral barriers in FRC-PBD allows for complete resolution of the Johari-Goldstein β-process from the primary α-process in the simulation time window. We find that relaxation in the β-regime occurs as the result of large-angle excursions of all backbone dihedrals that are largely decoupled from the dynamics of the polymer matrix, while the α-relaxation exhibits strong coupling between matrix motion and polymer dihedral relaxation.

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