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Coarse grain modeling of the high-rate stress-strain behavior for select model Poly[urethane urea] (PUU) elastomers T.L. CHANTAWANSRI, Y.R. SLIOZBERG, A. HSIEH, J.W. ANDZELM, Army Research Laboratory — Microphase-separated PUU, which consists of 4,4'-dicyclohexylmethane diisocyanate, diethyltoluenediamine and poly[tetramethylene oxide](PTMO), exhibits versatile mechanical properties making them an excellent choice for potential applications in the form of films, adhesives, coatings and matrix materials for composites. To elucidate the effects of composition, including the hard segment content & molecular weight of PTMO, on rate-dependent mechanical deformation in the high strain-rate regime ($>> 10^5$/s) the stress-strain behavior for PUU at various rates are calculated for four model systems using a coarse-grain model. Pair interactions between topologically non-connected particles are described by the standard truncated Lennard-Jones (LJ) pair potential, where bonded particles interact according to the standard FENE/LJ potential. An angle harmonic potential is also used to enforce the rigidity of the hard segments, and the system is evolved using molecular dynamics. Stress-strain curves are calculated at various strain-rates and qualitatively agree with experimental results when extrapolated to higher rate. Further analysis of the morphology is also performed to characterize the morphology and discern its connection to the calculated mechanical properties.

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