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Viscoelasticity of crosslinked epoxy networks under extreme conditions from molecular dynamics simulation TIMOTHY SIRK, US Army Research Laboratory, MIR KARIM, KETAN KHARE, RAJESH KHARE, Department of Chemical Engineering, Texas Tech University, JAN ANDZELM, US Army Research Laboratory — Understanding viscoelastic behavior at ballistic conditions is critical for the design of new polymeric-based protective materials in civilian and military applications. The relaxation mechanisms available to polymer networks at ballistic conditions (strain rate $>10^5$ s^{-1}) include both segmental and chain relaxations, and thus cannot be understood as a simple superposition of the relaxations acting at the much lower strain rates typically considered in experiments. We present viscoelastic properties of polymer networks found from atomistic molecular dynamics simulation, where we consider an epoxy monomer, di-glycidyl ether of bisphenol A, reacted with binary amine mixtures, 4,4'-methylenebis(cyclohexylamine) and poly(oxypropylene) diamine. Our results show that (1) oscillatory strain simulations similar to experimental dynamic mechanical analysis are capable of predicting the complex modulus at high frequencies, (2) the maximum of the loss modulus can be expected to occur well-above the glass transition temperature predicted by simulated volumetric data, and (3) the molecular weight between crosslinks strongly influences the thermodynamic state required for ideal energy dissipation. These results from oscillatory strain will also be compared with other methods of evaluating linear viscoelasticity from molecular dynamics simulation.

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