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Dynamic Deformation of Thermosetting Polymers—All Atomistic Simulations MESFIN TSIGE, Department of Polymer Science, The University of Akron, Akron, OH, NATALIA SHENOGINA, SHARMILA MUKHOPADHYAY, Department of Mechanical and Materials Engineering, Wright State University, Dayton, OH, SOUMYA PATNAIK, Propulsion Directorate, Air Force Research Laboratory, Dayton, OH — We are using all-atom molecular dynamics simulations to investigate the interconnection between structural and mechanical properties of highly cross-linked polymer networks. In this study we focused on the widely used resin-hardener system composed of DGEBA epoxy oligomers and aromatic amine hardener DETDA. Accurate cross-linked models were developed using the effective cross-linking procedure that enables to generate thermoset structures with realistic structural characteristics. These models were used to examine the elastic properties of thermosetting networks with various degrees of curing and length of resin strands both in glassy and rubbery states. In our recent study we employed static deformation approach to estimate potential energy contribution to the mechanical response. In the present work we are using dynamic deformation approach which takes into account both potential energy and thermal motions in the structure. Uniaxial, volumetric and shear dynamic deformation modes were used to obtain Young's, bulk, shear moduli and Poisson's ratio directly. We also calculated elastic constants using formulae of linear elasticity and analyzed the results obtained by direct deformation and interconversion methods. The elastic properties determined from these two approaches are in good agreement with each other and also with experimental data.

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