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**Molecular dynamics simulations of highly cross-linked polymer networks: prediction of thermal and mechanical properties** NATALIA SHENOGINA, Wright State University, Dayton, OH, MESFIN TSIGE, University of Akron, Akron, OH, SHARMILA MUKHOPADHYAY, Wright State University, Dayton, OH, SOUMYA PATNAIK, Wright-Patterson Air Force Base, Dayton, OH — We use all-atom molecular dynamics (MD) simulations to predict the mechanical and thermal properties of thermosetting polymers. Atomistic simulation is a promising tool which can provide detailed structure-property relationships of densely cross-linked polymer networks. In this work we study the thermo-mechanical properties of thermosetting polymers based on amine curing agents and epoxy resins and have focused on the DGEBA/DETDA epoxy system. At first we describe the modeling approach to construction of realistic all-atom models of densely cross-linked polymer matrices. Subsequently, a series of atomistic simulations was carried out to examine the simulation cell size effect as well as the role of cross-linking density and chain length of the resin strands on thermo-mechanical properties at different temperatures. Two different methods were used to deform the polymer networks. Both static and dynamic approaches to calculating the mechanical properties were considered and the thermo-mechanical properties obtained from our simulations were found in reasonable agreement with experimental values.

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[X] Prefer Oral Session
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