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**Molecular Modeling of Thermosetting Polymers** SOUMYA PATNAIK, Air Force Research Laboratory, VIKAS VARSHNEY, Universal Technology Corporation, BARRY FARMER, Air Force Research Laboratory — In this work we present molecular modeling of thermosetting polymers with special emphasis on building atomistic models. Different approaches to building highly cross-linked polymer networks starting from un-crosslinked systems are discussed. A multi-step procedure for relaxing the molecular topology during crosslinking was proposed which allows for minimizing the increase in the residual internal stresses with increasing degree of crosslinking. This methodology was applied to epoxy based thermosets and several materials properties such as density, Young's modulus, glass transition temperature, thermal expansion coefficient and volume shrinkage during curing were calculated and found to be in good agreement with experimental results. Along with the materials properties, the simulations also highlighted the distribution of molecular weight build up and inception of gel point during the network formation.

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