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MD simulations of chemically reacting networks DANA ROTTACH, University of New Mexico, JOHN CURRO, AIDAN THOMPSON, GARY GREST[1], Sandia National Laboratories — The aging of polymeric networks is difficult to investigate in the laboratory. Chemical control is at the mercy of nature, and resulting network structures aren't easily observable. Molecular dynamics simulations, without these limitations, are used to perform virtual stress relaxation and permanent set measurements. Tobolsky's Independent Network Model (INM) and Flory's modifications are tested. The INM states that crosslinks added to an existing network can be treated as forming a second, parallel network. Simulations of these two-stage systems support this model. Flory hypothesized that the effect of removing first stage crosslinks is reduced by an effective switching of second-stage crosslinks. This is supported by simulations in which all first-stage crosslinks are removed. Tobolsky and Flory assumed Gaussian network segments and, more problematically, affine deformation in the derivation of quantitative relationships for the INM. The simulation results match their predictions only qualitatively. More advanced models of elasticity are discussed.

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