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Coarse grain modeling of imperfect networks and gels YELENA SLIOZBERG, TANYA CHANTAWANSRI, TIMOTHY SIRK, JAN ANDZELM, RANDY MROZEK, JOSEPH LENHART, U.S. Army Research Laboratory — There is a strong interest in chemically and physically cross-linked entangled polymer networks and gels due to their tailorability in respect to both mechanical and structural properties. Even so, these properties are sensitive to imperfections in the polymer networks, such as dangling ends and loops. Computational modeling is a viable tool to understand the effects of these imperfections on properties in a controlled environment, in which specific defects can be systematically created and varied. In this study, we have employed generic bead-spring models of flexible chains to study a chemically and physically cross-linked network. Our results will show the importance defects, such as dangling ends and loops, on the mechanical and structural properties of these networks. We will also discuss the effects of these defects on the time-dependent elastic modulus. The simulation results qualitatively agree with experimental results and the other theoretical predictions.

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