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Reactive MD simulations of deformation and failure in cross-linking polymers. CHANDRASHEKAR SHANKAR, JOHN KIEFFER, University of Michigan — We have developed a computational framework for studying the behavior of polymer systems simultaneously undergoing strain deformations and polymerization reactions, such as epoxy resins and other reacting polymeric systems. Using our simulations we predict system properties, such as yield strength, toughness and ultimate failure of the system at various stress regimes, and examine how these properties are affected by variations in reaction rates and curing conditions. Accordingly, we use this framework to optimize the design of autonomously healing polymer matrix composites, containing di-cyclo-penta-diene (DCPD) as the healing agent. Polymerization reactions occur on time scales, currently inaccessible by conventional MD. We bridge this chasm by coarse graining real monomers as soft interacting beads. Timescale mapping between the coarse-grained simulations and a reactive MD model of atomically detailed systems with reacting monomers such as DCPD, is achieved using diffusion timescale matching. Reaction processes in the coarse-grained simulations are accounted by a MC scheme, in which we can adjust the probability of reaction and the geometric aspects reflecting the reaction mechanisms in a particular polymer system.

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