PHANTOM CHAIN SIMULATIONS FOR TETRA AND TRI-BRANCHED NETWORKS

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Effects of branch functionality on mechanical properties of polymer networks have not been fully elucidated yet, although multi-functional approaches have been mainly attempted. For instance, Fujiyabu et al.[1] have recently reported that polymer networks made from tri-branch prepolymers exhibit superior mechanical properties to tetra-branch analogs. Although they attribute the difference to stretch-induced crystallization observed in tri-branch poly (ethylene glycol) networks, the mechanism still needs to be clarified. In this study[2], we performed coarse-grained molecular simulations to extract the effect of branch functionality. The prepolymers were replaced by bead-spring phantom chains, and gelation was simulated by a Brownian dynamics scheme[3,4] We subjected the resultant networks to energy minimization and uniaxial stretch by introducing breakage for elongated segments. In the stress-strain relation thus obtained, stress and strain at the break were larger for tri-branch networks than for tetra-branch analogs, consistent with the experiment. The superiority of tri-branch networks is observed in a wide range of the conversion ratio in gelation, molecular weights of prepolymers, and polymer concentrations. The result implies that the mechanical superiority of tri-branch networks to tetra-branch ones is due to a fundamental structural difference generated during gelation.

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