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Three-dimensional computational model of self-reinforcing polymer gels SANTIDAN BISWAS, VICTOR V. YASHIN, ANNA C. BALAZS, Univ of Pittsburgh — We utilize the gel lattice-spring approach to develop the 3D computational model of polymer gels that become stronger and tougher in response to a mechanical deformation. The polymer chains are assumed to incorporate the folded domains that encompass the reactive functional groups (cryptic sites). Under deformation, the domains unfold and expose the cryptic sites, which can then form labile bonds with the linker chains grafted to the network. Once the deformation is removed, the linkers detach from the cryptic sites, and unfolded domains go back to the folded configuration thus hiding the cryptic sites. The gel behavior under applied force is described by the equations of elasticity of the polymer network coupled to the kinetic equations for the folding and binding transitions. The model equations take into account the effects of finite chain extensibility on the gel elasticity and mechanosensitive reaction rates. Elasticity of the transient network is described using the Flory model. The developed 3D computational model could be used for designing novel polymer gel-based materials that exhibit self-strengthening under deformation.

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