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Modeling heterogeneous polymer-grafted nanoparticle networks having biomimetic core-shell structure BADEL L. MBANGA, VICTOR V. YASHIN, Chemical Engineering Department, University of Pittsburgh, Pittsburgh, PA 15261, USA, NIELS HOLTEN-ANDERSEN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh, Pittsburgh, PA 15261, USA — Inspired by the remarkable mechanical properties of such biological structures as mussel adhesive fibers, we use 3D computational modeling to study the behavior of heterogeneous polymer-grafted nanoparticle (PGN) networks under tensile deformation. The building block of a PGN network is a nanoparticle with grafted polymer chains whose free ends' reactive groups can form both permanent and labile bonds with the end chains on the nearby particles. The tunable behavior of cross-linked PGN networks makes them excellent candidates for designing novel materials with enhanced mechanical properties. Here, we consider the PGN networks having the core-shell structures, in which the type and strength of the inter-particle bonds in the outer shell differ from those in the core. Using the computer simulations, we obtain and compare the ultimate tensile properties (strength, toughness, ductility) and the strain recovery properties for the uniform samples and various core-shell structures. We demonstrate that the core-shell structures could be designed to obtain highly resilient self-healing materials

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