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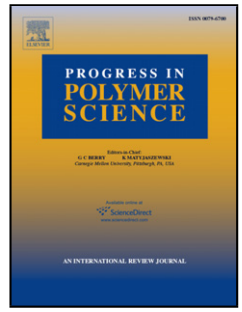

Title: Ductility, toughness and strain recovery in self-healing dual cross-linked nanoparticle networks studied by computer simulations

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Review

Ductility, toughness and strain recovery in self-healing dual cross-linked nanoparticle networks studied by computer simulations

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ABSTRACT

One of the challenges in formulating useful nanocomposites is creating materials that are both tough and strong. Here, we review results of computational studies on a new class of nanocomposites that exhibit these desirable properties. The fundamental unit in these materials is a polymer grafted nanoparticle (PGN), which encompasses a rigid core and a corona of end-grafted polymers. We focus on a concentrated solution of these PGNs; the solution is assumed to be a good solvent for the grafted chains, which are in the semi-dilute regime. The free ends of the grafted chains encompass chemically reactive groups. Hence, with the overlap of the coronas on neighboring nanoparticles, the reactive end groups can form labile or more stable ("permanent") bonds, leading to the creation of a "dual cross-linked" network. To predict the mechanical properties of these dual cross-linked PGN networks, we developed a multi-scale model that captures interactions occurring over the range of length and time scales that characterize the performance of the system. Namely, the model integrates the essential structural features of the polymer grafted nanoparticles, the interactions between the overlapping coronas, the kinetics of bond formation and rupture between the reactive end-groups and the response of the entire sample to mechanical deformation. Using this computational approach, we determined the effect of the labile bond