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Modeling heterogeneous polymer-grafted nanoparticle networks
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Via a dynamic 3D computational approach, we simulate the heterogeneous polymer-grafted nanoparticle networks. The nanoparticles rigid cores are decorated with a corona of grafted polymers, which contain reactive functional groups at the chain ends. With the overlap of grafted polymers, these reactive groups can form weak labile bonds, which can reform after breakage, or stronger bonds, which rupture irreversibly and thus, the nanoparticles are interconnected by dual cross-links. Previous work has been done on homogeneous networks, while we introduce the heterogeneity by considering two types of particles having different reactive functional groups, so that the labile bond energy varies depending on types of the two end reactive groups. We study the effect of tensile and rotational deformations on the network morphology, and observe, in particular, the phase separation of two types of particles. Our results will provide guidelines for designing transformable material that can controllably change structure under mechanical action.

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