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Molecular Dynamics Simulations on the Mechanical Properties of Blend of Polymer and Polymer Grafted Nanoparticles DONG MENG, SANAT KUMAR, Columbia University, GARY GREST, Sandia National Laboratories, TING GE, MARK ROBBINS, The Johns Hopkins University — Grafting polymers onto the surface of NPs has become one of the most effective approaches to integrate NPs into polymer melts. It then becomes crucial to be able to understand the mechanical properties of the resulting composites. Using molecular dynamics simulations we investigated how the presence of grafted NPs changes mechanical responses of an entangled polymer matrix below its glass transition temperature under uniaxial tensile deformation. It is found that comparing to neat polymer melts adding fillers slightly increases the elastic modulus as well as the yielding stress of the composites. But changes in the fracture work (total work needed to pull samples to failure) are every dependent on the loading fraction and dispersion state of NPs in polymer matrix. At small loadings fracture work is found to be significantly reduced due to polymer crazing around NPs, which is induced by local triaxial stresses, while at higher loadings a big degree of enhancement is observed because of network forming among grafted NPs.

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