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Effect of Grafting Density and Curvature of Nanoparticle on Mechanical Properties of Polymer Nanocomposite HUIKUAN CHAO, ROBERT RIGGLEMAN, Department of Chemical and Biomolecular Engineering, University of Pennsylvania — Polymer nanocomposites (PNCs) are materials obtained by dispersing nanoparticles in a polymer matrix. Due to the large surface-to-volume ratio between the nanoparticles and the polymer, substantial enhancement in dynamic and mechanical properties can be observed for relatively low concentrations of particles. One common approach for ensuring dispersion of the nanoparticles is to end-graft polymers that are miscible in the host polymer matrix to the surface of the nanoparticles in the PNC. In many applications, understanding the role that the nanoparticles with grafted chains have on the resulting mechanical properties of the PNC will be of central importance in the final applications as well as the processing of the original sample. In this talk, I will first introduce the coarse grain model we used to study various mechanical properties of polymer and PNC. By designing a model system where the nanoparticles with different radii are remain dispersed whether they are grafted with polymer chains or not, we are able to isolate the role that chain grafting has on various aspects of the mechanical response of the PNC. We provide a detailed picture of how the elastic constants, yield stress, and the strain hardening behaviors depend on the grafting density and the size of nanoparticles

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