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Nanoparticle Alignment and Repulsion During Failure of Glassy Polymer Nanocomposites ALFRED CROSBY, JONG-YOUNG LEE, QINGLING ZHANG, TODD EMRICK, University of Massachusetts Amherst — We investigate crazing and failure in a model nanocomposite of surface modified nanoparticles (cadmium selenide, diameter is 5 nm) blended into polystyrene. We demonstrate that nanoparticles undergo three stages of rearrangement during craze formation and propagation in glassy polymer nanocomposites: 1) Alignment along the precraze, 2) Expulsion from craze fibrils, and 3) Assembly into clusters entrapped between craze fibrils. At an optimal volume fraction of nanoparticles, the failure strain of the nanocomposite is increased by nearly 100% relative to unfilled polystyrene. This optimal volume fraction is related to the balance of two mechanisms: 1) the decrease in cross-tie fibril density for craze structures, and 2) the decrease in the probability of craze widening at higher tensile strain by decreasing the number of polymer entanglements at small interparticle lengths. These results offer a clear and detailed understanding of failure mechanism of glassy polymer-nanoparticle composites, and provide predictions for the future design of nanoparticle-based materials.

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