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The Effect of Nanoparticle Shape on Polymer-Nanocomposite Rheology and Tensile Strength SCOTT T. KNAUERT, Physics Department Wesleyan University, JACK F. DOUGLAS, Polymers Division National Institute of Standards and Technology, FRANCIS W. STARR, Physics Department Wesleyan University — We investigate how nanoparticle shape influences the melt shear viscosity η and the tensile strength τ , with a focus on fullerene, carbon nanotube, and clay sheet nanocomposites. We simulate model nanoparticle dispersions of icosahedral, tube or rod-like, and sheet-like nanoparticles, all at a volume fraction ≈ 0.05 . Our results indicate an order of magnitude increase in the viscosity η relative to the pure melt. This finding can not be explained by continuum hydrodynamics and we provide evidence that the η increase has its origin in chain bridging between the nanoparticles. We find that this increase is the largest for the rod-like nanoparticles and least for the sheet-like nanoparticles. Curiously, the enhancements of η and τ exhibit opposite trends with increasing chain length N and with particle shape anisotropy. Evidently, the concept of bridging chains alone cannot account for the increase in τ and we suggest that the deformability or flexibility of the sheet nanoparticles contributes to nanocomposite strength and toughness by reducing the relative value of the Poisson ratio of the composite.

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