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Particle inclusion effect on the rheological properties of polymeric materials GREGORY TOEPPERWEIN, GEORGE PAPAKONSTANTOPOULOS, JUAN DE PABLO, University of Wisconsin — Recently developed algorithms have permitted the extraction of the primitive path and the entanglement length, Ne, from simulations of polymer melts. Experimental studies on the effect of the addition of nanoparticles to a polymer melt have revealed that nanoparticles can alter the plateau modulus and subsequently the entanglement length of the polymer. We use simulations to directly estimate the entanglement length of nanocomposite systems to study the effect of spherical and anisotropic nanoparticles on the entanglement length of a polymer matrix. In this work we present a systematic study of the effects of particle-polymer interactions, particle size, aspect ratio and volume fraction. Advanced Monte Carlo techniques involving chain connectivity algorithms are used to create statistically independent configurations. Attractive, neutral and repulsive polymer particle interactions are considered. Furthermore, we examine the effect of different assumptions on the calculation of Ne.

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