Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Mechanisms of Steady State Rheological Behavior of Polymer Nanoparticle Composites VICTOR PRYAMITSYN, VENKAT GANESAN, University of Texas at Austin — We use a mesoscale computer simulation framework to delineate the the mechanisms behind the linear and nonlinear dynamical properties of polymer-nanoparticle composites. Our studies specifically focus on the regimes where the particle sizes and the interparticle distances become comparable to the polymer sizes. Our results indicate that the zero shear viscosities of the composite can be described in a manner similar to colloidal suspensions in a simple fluid when both the particle-induced changes in the polymer relaxation spectra and the polymer slip effects are accounted. The nonlinear shear rheology and the first normal stresses of the composite exhibits a subtle interplay between the shear thinning arising from the polymer and particle stresses. Overall, at dilute and semidilute nanoparticle concentrations, the composite shear rheology is dominated by the shear thinning of the polymer chains which in turn is modified by the presence of the particles. For higher particle loads, especially in regimes where particle jamming manifests, the polymeric contribution to the rheology becomes much less important and the shear thinning is dominated by the particles stresses. These competing efffects lead to intriguing polymer molecular weight, particle loading dependencies for the steady shear rheological behavior. Our results and mechanistic explanations are in excellent agreement with associated experimental observations.

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Date submitted: 11 Jan 2006 Electronic form version 1.4