Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Influence of nanorods on the properties of polymeric materials GREGORY N. TOEPPERWEIN, ROBERT A. RIGGLEMAN, JUAN J. DE PABLO, University of Wisconsin — Nanoscopic additions, such as metallic nanoparticles or carbon nanotubes, can dramatically impact the mechanical properties of polymeric materials, such as the plateau modulus, which is intimately related to the entanglement length of the polymer. To explore the connection between nanocomposite configurations and the dynamic mechanical effects that are difficult to probe experimentally, due to challenges associated with sample preparation and particle dispersion, we have performed extensive Molecular Dynamics and Monte Carlo simulations of polymer nanocomposites with nanoparticles whose size, shape, and concentration have been varied systematically. Calculations of the entanglement network through primitive path analysis of these composites have enabled us to connect nanorod effects on the entanglement network structure and density to the system's dynamic properties. The main outcome of our study is a better understanding of how inclusions alter entanglements and how those entanglements are magnified in macroscopic observables.

Gregory Toepperwein
University of Wisconsin

Date submitted: 20 Nov 2008 Electronic form version 1.4