Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Nanoparticle effect on polymer chain dynamics and entanglement network[1] YING LI[2], University of Connecticut, MARTIN KROGER, ETH Zurich — We investigated structure and dynamics of polymer nanocomposites through molecular modeling, by considering different molecular weights of polymers chains, and volume fractions of fillers. The dynamics of unentangled chains can be separated into two phases, a bulk polymer phase and a confined polymer phase between fillers. The dynamics of a confined polymer is slower than that of a bulk polymer, while still exhibiting high mobility. The amount of the bulk polymer phase is found to exponentially decay with increasing volume fraction of fillers. When highly entangled polymer chains are confined between fillers, their conformation and entanglement network are dramatically changed, in district with their unentangled counterparts. The entangled polymer chains are found to be significantly disentangled and flattened during increment of the volume fractions of spherical nonattractive fillers. A critical volume fraction is found to control the crossover from polymer chain entanglements to 'nanoparticle entanglements', below which the polymer chain relaxation accelerates upon filling. These results provide a microscopic understanding of the dynamics of entangled polymer chains inside their composites, and offer an explanation for the unusual rheological properties of polymer composites.

[1]Supported by Department of Mechanical Engineering, University of Connecticut
[2]Membership Pending

Ying Li
University of Connecticut

Date submitted: 06 Nov 2015 Electronic form version 1.4