Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Molecular Dynamics Simulation on Rheological and Dyanmics Properties of Polymer Nanocomposite System With Thermal Stiffening Behaviors[1] WEI PENG, RAHMI OZISIK, PAWEL KEBLINSKI, Rensselaer Polytechnic Institute — The rheological and dynamic properties of polymer nanocomposite systems were studied via Molecular Dynamics (MD) simulations. The current study was inspired by Senses et al. (Senses, E.; Isherwood, A.; Akcora, P. ACS Appl. Mater. Interfaces 2015, 7, 14682), where a reversible thermal stiffening behavior was observed in nanocomposite polymers, in which the matrix chains and surfactant polymer chains on the nanofillers showed 200 C difference in their glass transition temperatures (Tgs). The simulated systems contained nanoparticles that were grafted with high-Tg chains mixed within a matrix of low-Tg flexible chains. The rheological and dynamic properties of this polymer nanocomposite system with two distinct morphologies, stretched and collapsed, were studied. In stretched morphology, the grafted chains were well dispersed within the matrix, whereas in the collapsed morphology, the grafted and the matrix chains were phase separated. Non-equilibrium MD simulation results showed that stretched systems had significantly greater storage modulus than collapsed ones. The effects of chain length and volume fraction of grafted chains were further investigated to study the mechanism of the stiffening observed in the stretched nanocomposite.

[1]This material is based upon work supported by NSF under Grant No. CMMI-1538730

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Date submitted: 11 Nov 2016 Electronic form version 1.4