Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Glass Transitions in Polymer Nanocomposites DONG MENG, SANAT KUMAR, Columbia University — For polymers are under geometric confinement, it is generally believed that the glass transition temperature (T_g) increases with favorable interfacial interactions. Experiments [1] and simulations [2] have reported that T_g increases almost proportionally to the attractive polymer-surface interactions. However, recent studies [3,4] have reported the contradictory finding that the T_g shift is rather modest and insensitive to the strength of interfacial attractions. In this study, we investigate the glass transition in polymer nanocomposites using molecular dynamics simulations. With attractive polymer-nanoparticle (NP) interactions, we find that T_g is increased by $\sim 3\%$ at moderate loadings and that the shift stays almost unchanged when the polymer-NP attractions are further increased by one order of magnitude. Both are in agreement with the recent experiments at comparable NP loadings [4]. We show that this is because the strongly adsorbed polymer segments do not participate in the glass transition. In other words, strong polymer-NP attractions create immobile polymer "coatings" around NPs that shield them from direct contact with the mobile polymers.

[1] Tate, R. S.; de Pablo, J. J.; Nealey, P. F. Journal of Chem. Phys. 2001, 115 (21), 9982-9990.
[2] Torres, J. A.; Nealey, P. F.; de Pablo, J. J. Phys. Rev. Lett. 2000, 85 (15), 3221−3224.
[3] Lu, H. Y.; Chen, W.; Russell, T. P. Macromolecules 2009, 42 (22), 9111−9117.
[4] Moll, J.; Kumar, S.K. Macromolecules 2012, 45 (32), 1131−1135.

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Date submitted: 15 Nov 2013 Electronic form version 1.4