Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Molecular Dynamics Simulations to Determine the Effects of Copolymer Architecture and Nanofiller Adsorption Strength on Viscoelastic Properties of Polymer Nanocomposites ALEX TRAZKOVICH, The Ohio State University and Cooper Tire and Rubber Company, LISA M. HALL, The Ohio State University — We simulate a simple nanocomposite consisting of a single spherical nanoparticle surrounded by coarse-grained polymer chains. The polymers are composed of two different monomer types, which have different interaction strengths with the nanoparticle. We examine the effect of copolymer sequence and monomer-nanoparticle interaction strength on structure (using the monomer-nanoparticle radial distribution function) and chain relaxation times (using the polymer end-to-end vector autocorrelation function). We also examine relaxations times as a function of distance from the nanoparticle surface in order to understand the effect of copolymer sequence on the range and magnitude of the interphase of slowed dynamics surrounding the nanoparticle. Finally, we use the stress autocorrelation function to calculate the dynamic storage and loss modulus, which we also measured as a function of copolymer sequence, monomer-nanoparticle interaction strength, and distance from the nanoparticle surface. Our work is motivated by tire tread compounds, which are composed primarily of styrene-butadiene rubber copolymer (with potentially controllable block structure) and reinforced with carbon black and/or silica nanoparticles. Our focus on local properties near the nanoparticle surface is expected to reveal trends that are applicable to the bulk properties of these systems.

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Date submitted: 11 Nov 2016 Electronic form version 1.4