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Molecular Dynamics Simulations of Silica-Filled Copolymers with Variable Sequence for Applications in Tire Treads ALEX J. TRAZKOVICH, The Ohio State University and The Cooper Tire and Rubber Company, LISA M. HALL, The Ohio State University — We simulate a simple nanocomposite relevant to tire tread compounds 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. The monomer sequence can be varied to model different copolymer configurations. We study the polymer end-to-end vector autocorrelation functions to obtain relaxation times of adsorbed and bulk polymer, showing how the interphase is affected by the polymer type and the monomer-nanoparticle interaction strengths. An understanding of the effect of copolymer sequence on the range of the polymer interphase and the magnitude of the effect on chain dynamics is critical to tire tread material design since the primary polymer component of modern tire tread is styrene-butadiene rubber (SBR) copolymer, which may be synthesized in primarily random or in various blocky copolymer configurations. Macromolecular adsorption to and desorption from filler surfaces has a significant effect on hysteresis, and in tire treads, hysteresis must be controlled to optimize the tradeoff between traction and rolling resistance. Superior tire tread materials must have high hysteresis under the operating conditions of traction while maintaining low hysteresis under the operating conditions of rolling resistance. An opportunity exists to control hysteresis through the use of SBR with specific monomer sequences.

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