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Influence of Nanoparticles on the Amplitude of Molecular Motions and the Fragility a Model Glass-Forming Polymer Melt. JACK DOUGLAS, polymers Division, National Institute of Standards and Technology, FRANCIS STARR, Department of Physics, Wesleyan University — We investigate the impact of the addition of nanoparticles on both the fast and slow dynamics of a coarse-grained polymer fluid by molecular dynamics. The fast dynamics is characterized by the Debye-Waller factor (the average mean square particle displacement at a characteristic time in the caged particle motion regime) and the slow structural relaxation is characterized by the coherent intermediate scattering function. Our study explores how both the polymer-particle and nanoparticle volume fraction change the amplitude of the high frequency molecular motions (relative to the pure melt reference condition) and the strength of the temperature dependence of the structural relaxation time (defining the fragility of glass formation, as well as the glass transition temperature). Substantial variations of the Debye-Waller factor are observed and we test the effectiveness of the Buchenau relation linking the Debye-Waller factor to the long time structural relaxation time. We also consider how the presence of nanoparticles in the polymer melt influence the fragility of glass formation, where a range of criteria are utilized to define fragility. Appreciable changes of fragility are observed, these changes being dependent on the nanoparticle concentration and particle-polymer interaction.

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