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Modifying Fragility and Length Scales of Polymer Glass Formation with Nanoparticles BEATRIZ A. PAZMINO, Physics Dept., Wesleyan University, Middletown, CT, JACK F. DOUGLAS, Polymer Division, NIST, Gaithersburg, MD, FRANCIS W. STARR, Physics Dept., Wesleyan University, Middletown, CT — We investigate the effects of nanoparticles on glass formation in a model polymer melt by molecular dynamics simulations. The addition of nanoparticles allows us to change the glass transition temperature T_g , the fragility of glass formation, and both static and dynamical length scales in a controlled fashion. We contrast the length scales of static density changes with the length scale over which nanoparticles perturb the dynamics, as well as the length scale of cooperative string-like motion. Using the Adam-Gibbs approach, we show how the changes of fragility can be interpreted as a measure of the scale of cooperative string-like motion. We contrast the behavior along isobaric and isochoric paths to T_g , and find that changes along an isobaric path (most relevant experimentally) are much smaller than those along an isochoric path.

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