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Dynamics of Vapor-Deposited Polymer Glasses from Simulation[1]
WENGANG ZHANG, FRANCIS STARR, Wesleyan University, JACK DOUGLAS, National Institute of Standards and Technology — We use molecular dynamics simulations to mimic the physical vapor deposition of glassy polymer films. Like experiments, the deposition results in "ultrastable glasses" that have lower energies, and greater kinetic stability than ordinary glasses. It has been suggested that these ultrastable glasses may be equivalent to very highly aged ordinary glasses. To explore this possibility, we contrast both the structure and dynamics of deposited and ordinary glasses. Our modeling indicates that the deposited polymer glass is structurally distinct from the ordinary glass due to anisotropy of chain packing. If the deposited glasses correspond to highly aged ordinary glasses, we would expect vastly larger relaxation times for the deposited glass. Instead, we find that relaxation times of the vapor-deposited glass are nearly the same as that of the ordinary glass. These findings do not support the view that vapor-deposited glassy polymer films are equivalent to highly-aged ordinary glassy polymer films. We further study the dynamical heterogeneity of highly out-of-equilibrium polymer films.

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