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Glass formation behavior of an isolated polymer chain[1] WESTON MERLING, JACK MILESKI, DAVID SIMMONS, University of Akron — A single polymer chain in isolation logically represents the extreme limit of nanoconfinement with respect to segmental dynamics and glass formation. Work in thin polymer films suggests that one should expect a large Tg suppression in such systems. However, recent dielectric relaxation measurements of isolated chains of P2VP on a silica substrate found bulk-like Tg in this system, apparently raising questions about the nature of observed nanoconfinement effects on the glass transition. Here we describe simulations of glass formation in an isolated polymer chain, both free-floating and deposited on a substrate. Results indicate that free-floating isolated polymer chains exhibit a depression in the dynamic glass transition temperature equivalent to more than 100K in polystyrene units. However, when a chain is deposited on a substrate with sufficiently favorable surface interactions, bulk-like dynamics can be recovered due to competition between the free-surface and adsorbed interface. When this compensation effect is taken account, these results indicate that the observation of bulk-like dynamics in isolated P2VP chains on a silica substrate is consistent with observations of large Tg suppressions in polymer films supported by less attractive substrates.

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