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Molecular simulations of confined polymer glasses ROBERT RIGGLEMAN, AMIT SHAVIT, University of Pennsylvania — For many technological applications ranging from semiconductor manufacturing to membranes for separations and flexible displays, the properties of glass-forming materials confined on the nanoscale are of critical importance. For example, common semiconductor manufacturing techniques rely on the mechanical integrity of amorphous polymer nanostructures. Experiments over the past several years have demonstrated that many of the properties of polymer glasses (e.g., the glass transition temperature, Tg, and the elastic constants) can change significantly and in unintuitive ways when confined to dimensions below approximately 100 nm. These confinement effects depend strongly on the detailed polymer chemistry. In this talk, I will describe our recent work using molecular simulations to study the effects of nanoscale confinement on both the dynamic and mechanical properties of a series of coarse-grained polymer models. Our coarse-grained models systematically explore the effects of polymer chemistry by gradually changing the polymer backbone stiffness and analyzing changes in various properties in free-standing thin films. We find that the confinement effects can vary drastically depending on the properties measured, and in some cases we observe significant ordering of our polymer chains

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