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Simulations of grafted and ungrafted polymeric films near the glass transition REGINA BARBER-DEGRAAFF, ARLETTE BALJON, Dept. of Physics, San Diego State University, RAJESH KHARE, Dept. of Chemical and Biological Eng, U. of Wisconsin — Glass transition behavior of ultrathin polymer films is investigated by means of molecular dynamics simulations. We study thin polymer films composed of bead-spring model chains and supported on an idealized lattice substrate surface. Experimentally, it has been found that the glass transition temperature (Tg) of such films rises sharply when a fraction of the polymer chains are grafted to the substrate. In this work, we investigate the impact of chain grafting, and the strength of polymer-surface interaction, on the film glass transition temperature. Three different methods - volumetric, energetic, and dynamic are used to determine the Tg of the films. Our results suggest the existence of two different transition temperatures: when the temperature of the melt film is lowered, a first transition, which is characterized by an anomaly in the heat capacity, occurs. Upon decreasing the temperature further, a point is reached at which the internal relaxation time of the film (as calculated from bead diffusion, for example) diverges. The former transition temperature appears to be related to the structural changes in the film, and in qualitative agreement with the experiments, shows a dependence on the characteristics of the polymer-surface interaction. By contrast, the latter temperature is independent of the strength of the polymer- surface interaction.

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