Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Local Dynamic Mechanical Properties of Model Free-Standing Polymer Thin Films KENJI YOSHIMOTO, TUSHAR JAIN, JUAN DE PABLO, University of Wisconsin - Madison — We present results that strongly support a heterogeneous distribution of dynamic mechanical properties (DMP) in model free-standing polymer thin films. While a number of groups are investigating the mechanical properties of glassy polymer thin films on a substrate, enhanced molecular-level understanding will be required to further rationalize their observations. This study highlights the free-standing geometry; we eliminate any convolution of effects arising from the presence of a free surface and a substrate. The local DMP are calculated from nonequilibrium MD simulations with a coarse-grained polymer model. Our simulation results suggest that the soft surface layers coexist with the bulk-like rigid regions in the thin films below the glass transition temperature (Tg). By increasing the temperature, we show that the thickness of the soft surface layers substantially increases. The overall stiffness of the free-standing films is thereby shown to be much smaller than that of the bulk. The molecular mechanism of surface softening is revealed by a normal mode analysis of the glassy thin films; large, cooperative motions of polymer segments are enhanced near the free surfaces in the vicinity of Tg.

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Date submitted: 01 Dec 2004 Electronic form version 1.4