Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Local dynamics of glass-forming polystyrene thin films from atomistic simulation YUXING ZHOU, SCOTT MILNER, The Pennsylvania State University — Despite a wide technological application ranging from protective coatings to organic solar cells, there still no consensus on the mechanism for the glass transition in polymer thin films a manifestation of the infamous glass problem under confinement. Many experimental and computational studies have observed a large deviation of nanoscale dynamical properties in thin films from the corresponding properties in bulk. In this work, we perform extensive united-atom simulations on atactic polystyrene free-standing thin films near the glass transition temperature and focus on the effect of free surface on the local dynamics. We study the segmental dynamics as a function of distance from the surface for different temperatures, from which relaxation time and thereby local T_g is obtained for each layer. We find the dynamics near free surface is not only enhanced but becomes less strongly temperature dependent as T_g is approached compared to the bulk. We find an increasing length scale associated with mobility propagation from the free surface as temperature decreases, but no correlation between local structure and enhanced relaxation rates near the surface, consistent with studies on bead-spring chains.

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Date submitted: 10 Nov 2016 Electronic form version 1.4