replacing MAR16-2015-007482. Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Sidechain Dynamics Explain Dissimilar Strength of Nanoconfinement Effect in Polystyrene and Poly(methyl methacrylate) Free Standing Thin Films[1] DAVID HSU, WENJIE XIA, JAKE SONG, SINAN KETEN, Northwestern University — Despite substantially similar bulk glass transition temperature (T_g) and other bulk properties, polystyrene (PS) and poly(methyl-methacrylate) (PMMA) exhibit characteristically different T_g depression in the free-standing ultrathin film configuration. The mechanism for this disparate T_g-nanoconfinement effect due to the free surfaces has not been fully explained. Here we utilize recently established chemically specific coarse grain (CG) models to qualitatively reproduce contrasting thickness dependent T_g and length scale of enhanced chain relaxation gradient in the interfacial layer. Vibrational mode analysis is utilized to uncover a relationship between the amplitude and frequency of sidechain fluctuations of reduced order models and the degree of T_g-nanoconfinement. By systematic variation of the distribution of mass in the sidechain versus the backbone, we demonstrate inertia-driven differences in sidechain fluctuations and T_g-nanoconfinement in the CG model. We hypothesize that mass distribution and sidechain flexibility are governing factors causing PS and PMMA free surface effect differences and also provide insight into broader nanoconfinement phenomena from past experiments.

[1] D.H., W.X., J.S., and S.K. acknowledge support by the University Partnership Initiative between Northwestern University and The Dow Chemical Company

David Hsu
Northwestern University

Date submitted: 06 Nov 2015 Electronic form version 1.4