Abstract Submitted
for the FWS16 Meeting of
The American Physical Society

Effect of the π-π interactions on the Glass Transition Temperature of Nanometer Thin Polystyrene Films GERARDO MENDOZA, San Diego State Univ, ALEXEY LYULIN, Eindhoven University of Technology, NIKOLAY BALABAEV, Institute of Mathematical Problems of Biology, ARLETTE BALJON, San Diego State Univ, CURTIS FRANK, DO YOON, Stanford University — The glass transition in free-standing films of linear and cyclic polystyrene (PS) was studied to identify a potential relationship between glass transition temperature (T_g) and film thickness. United-atom molecular-dynamic simulations were performed on free-standing films of varying thicknesses. Data revealed a positive correlation between T_g and film thickness, i.e. T_g decreases as film thickness decreases. At 20 nm the difference is less than 1%, while at 2.5 nm the difference is 13% for linear and 9% for cyclic chains. Recent studies show that a larger number of end groups inhabit the interface rather than the middle of the film and that a deficit of phenyl groups exists in the interfacial film layers nearly 1 nm below the surface. The large number of end groups would increase interfacial layer mobility while the deficit of phenyl groups would weaken the phenyl-phenyl aromatic (π-π) interaction. Through comparing the linear and cyclic PS, it was shown that cyclic chains lack end groups but the cyclic PS has an observed deficit of phenyl rings comparable to that in linear polymers. Therefore, the (π-π) interaction seems to be the reason for the observed T_g dependence on the thickness of thin PS films.

Gerardo Mendoza
San Diego State Univ

Date submitted: 01 Oct 2016 Electronic form version 1.4