Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

The Glass Transition in Ultra-Thin Polymer Filrms Confined between Structured Surfaces VIKRAM KUPPA, University of Cincinnati, GREGORY RUTLEDGE, MIT — Molecular Dynamics simulations are used to probe the structure and dynamics of polymers in ultra-thin slit pores. The simulation setup follows the structure of polymer nanocomposites, depicting chains intercalated between layered inorganic silicates. The structure and dynamics of bead-spring oligomers are studied for different film thicknesses, surface-segment interactions and temperature. In particular, we focus on the glass transition of the confined films as a function of layer thickness, interaction strength and density profiles: Tg is demonstrated to increase with confinement and attraction of the polymer with adjacent surfaces. The fragility of the polymer glasses is drastically different from the corresponding bulk system, and is shown to be dependent on the effective co-ordination number.

Vikram Kuppa
University of Cincinnati

Date submitted: 21 Nov 2008 Electronic form version 1.4