

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Molecular Simulation of Confined Polymer Films : Structure, Dynamics and the Glass Transition VIKRAM KUPPA, GREGORY RUTLEDGE, Massachusetts Institute of Technology — Molecular Dynamics simulations are used to probe the structure and dynamics of polymers in extreme confinements. The simulations mimic intercalated nanocomposites in which polymer chains are trapped in nanometer sized slit pores between layered inorganic surfaces : our system consists of thin films of bead-spring chains spatially restricted in one dimension by surfaces comprised of monomer beads arranged in an FCC configuration. The responses of the system are studied as a function of slit spacing, polymer-wall interaction strength and temperature. The glass transition temperatures, as well as the fragility of the confined films are seen to increase with increasing confinement and with increasing attraction of the polymer with the confining wall.

Vikram Kuppaa
Massachusetts Institute of Technology

Date submitted: 27 Nov 2007

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