Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Conformational Anisotropy and the Glass Transition in Polymer Thin Films FOLUSHO OYEROKUN, UCSB, ANNA CAVALLO, Uni-Mainz, MARCUS MUELLER, Uni-Gottingen, KENNETH SCHWEIZER, UIUC — A segmental level theory of the ideal kinetic glass transition, or dynamic crossover, temperature (T_c) in confined polymer films has been developed. The theory is based on an anisotropic generalization of a coarse grained polymer mode coupling theory which utilizes conformational and thermodynamic information from anisotropic PRISM theory and computer simulations. Confinement is found to enhance the bulk compressibility and induce anisotropic segmental dynamics. For non-capped films (free standing or supported films on neutral substrates) the theory predicts suppression of T_c, with confinement. The underlying mechanism is reduction of the degree of coil interpenetration and intermolecular repulsive contacts due to segmental scale alignment and deformation. The predicted suppression of T_c is nonuniversal and follows an inverse power law dependence on film thickness in reasonable agreement with experiments. For capped films simulations find a weak variation of the dimensionless compressibility with confinement suggesting little or no shift of T_g.

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Date submitted: 21 Nov 2005 Electronic form version 1.4