Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Glass transition temperature of PIB, PDMS and PMMA from small-time simulations[1] SOLOMON DUKI, Case Western Reserve University, MESFIN TSIGE, Southern Illinois University, PHILIP TAYLOR, Case Western Reserve University — We have applied some new techniques to obtain predictions of the glass transition temperatures T_g of poly(isobutylene), poly(dimethyl-siloxane), and poly(methyl methacrylate) from small-time atomistic molecular dynamics simulations. The different fragilities of these materials are reflected in the results of the simulations. One approach involved measurement of the apparent softening of the "cage" in which a monomer is bound, while another involved studying autocorrelation of a convolution of the velocity with a smoothing function in order to detect the frequency of escapes from the "cage." To check the accuracy of the short-time methods, the T_g of the polymers was also found using conventional diffusion simulations in which the rate of increase of the root mean squared displacement of an atom, monomer, or molecule is measured at very long times. The economical short-time simulations yielded results for T_g that were identical to those of the computer-intensive long-time simulations.

[1]Work supported by DOE Grant DE-FG02-05ER46244

Solomon Duki
Case Western Reserve University

Date submitted: 20 Nov 2008 Electronic form version 1.4