

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Monte Carlo Simulation of the Glass Transition in Polyethylene

RAJESH KHARE, Dept. of Chem. Engr., Texas Tech University, ORESTIS ALEXIADIS, VLASIS MAVRANTZAS, University of Patras, Greece, JOB BECKERS, ARLETTE BALJON, San Diego State University — The end-bridging (EB) Monte Carlo (MC) move has been used to simulate united atom models of bulk and end-grafted polyethylene both above and below the glass transition temperature (T_g). In previous work, EB move has been shown to lead to significant improvement in the relaxation of melts consisting of long polymer chains. We find that although a reasonable fraction of EB moves get accepted below glass transition in our MC simulation, the autocorrelation function of the chain end-to-end vector does not relax completely at these low temperatures. The temperature dependence of enthalpy and density is used to calculate the T_g for both bulk and thin film systems. For the film consisting of chains grafted on a hard surface, the T_g is slightly lower than that for the bulk, as expected in a system with unfavorable polymer-surface interactions.

Rajesh Khare
Texas Tech University

Date submitted: 20 Nov 2006

Electronic form version 1.4