Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Relaxation processes and glass transition in confined 1,4-polybutadiene films: A Molecular Dynamics study WOLFGANG PAUL, Martin-Luther-University, 55099 Halle, MATHIEU SOLAR, INSA, Strasbourg, France — We will present results from Molecular Dynamics simulations of a chemically realistic model of 1,4-polybutadiene (PB) chains confined by graphite walls. Relaxation processes in this system are heterogeneous and anisotropic. We will present evidence for a slow additional relaxation process related to chain desorption from the walls. We also study the structural relaxation resolved with respect to the distance from the graphite walls and show the influence of structural changes on the relaxation behavior. The temperature dependence of the dielectric relaxation in layers of different thickness near the walls shows no indication of a shift of T_g as a function of thickness when analyzed with a Vogel-Fulcher fit. We explain this by the importance of intramolecular dihedral barriers for the glass transition in PB which dominate over the density changes next to a wall except for a 1 nm thick layer directly at the wall.

Wolfgang Paul
Martin-Luther-University, 55099 Halle

Date submitted: 06 Nov 2015 Electronic form version 1.4