Molecular-dynamics simulations of thin films with a free surface
SIMONE PETER, HENDRIK MEYER, JOERG BASCHNAGEL, Institut Charles
Sadron — We present results [1,2] from molecular-dynamics simulations for a model
of non-entangled short polymer chains in a free standing and a supported film geom-
etry. We investigate the influence of confinement on static and dynamic properties
of the melt. We find that the relaxation at the surfaces is faster in comparison to
the bulk. We perform a layer-resolved analysis of the dynamics and show that it
is possible to associate a gradient in critical temperatures $T_c(y)$ with the gradient
in the relaxation dynamics. This finding is in qualitative agreement with experi-
mental results on supported polystyrene (PS) films [Ellison et al, Nat. Mater. 2,
695 (2003)]. Furthermore we show that the y-dependence of $T_c(y)$ can be expressed
in terms of the depression of $T_c(h)$, the global T_c for a film of thickness h, if we
assume that $T_c(h)$ is the arithmetic mean of $T_c(y)$ and parameterize the depression
of $T_c(h)$ by $T_c(h)=T_c/(1+h_0/h)$, a formula suggested by Herminghaus et al [Eur.
Phys. J E 5, 531 (2001)] for the reduction of the glass transition temperature in
supported PS films. We demonstrate the validity of this formula by comparing our
simulation results to results from other simulations and experiments.
[1] S. Peter, H. Meyer and J. Baschnagel, J. Polym. Sci. B, 44, 2951 (2006)
[2] S. Peter, H. Meyer, J. Baschnagel and R, Seemann, J. Phys: Condens. Matter
(2007)

Simone Peter
Institut Charles Sadron

Date submitted: 28 Nov 2006   Electronic form version 1.4