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MD study of polymer melts confined in thin films and nanopores

HENDRIK MEYER, Institut Charles Sadron, CNRS Strasbourg, France — The structure of chains is strongly affected if they are confined to films or pores smaller than the radius of gyration [1,2]. We report new molecular dynamics simulations of polymer melts confined between structureless walls comparing the thin film and pore confinement. It is shown that the form factor which is measured in scattering experiments is affected in a subtle way by the corrections to ideality [2]. The strong confinement reduces the number of overlapping chains and thus reduces entanglements. This leads to a clear acceleration in thin film confinement. For pore confinement, an acceleration is also found for intermediate pore diameters, but for extreme confinement, chains are segregated and they will block each other. [1] H. Meyer et al Eur. Phys. J. Sp.Top. 141 (2007) 167. [2] N. Lee et al EPL 93 (2011) 48002.

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