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Modeling Dielectric Relaxation in Simulations of Polymer Glasses and Thin Films HENDRIK MEYER, Institut Charles Sadron, CNRS UPR22, Strasbourg, France, SIMONE PETER, J. BASCHNAGEL — We perform molecular dynamics simulations to study the dielectric relaxation of a bead-spring model for a polymer melt in the bulk and in supported films [1]. By assigning dipole moments parallel and perpendicular to the backbone of all chains in the completed simulation trajectories we calculate the dielectric spectra of so-called type-A polymers which exhibit relaxation processes due to the local motion of chain segments ("segmental mode") and due to fluctuations of the end-to-end vector ("normal mode"). We find that the relaxation of both modes is enhanced in the films relative to the bulk. For the segmental mode this difference between film and bulk dynamics increases on cooling toward the glass transition. By a layer-resolved analysis of the segmental relaxation we show that the acceleration of the average film dynamics is a consequence of a smooth gradient in relaxation, originating from both interfaces where the segmental dipoles relax much faster than in the bulk.

[1] S. Peter et al Macromolecules 41 (2008) 7729.

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