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**Relaxation processes in polystyrene melts and ultra-thin films A.**

BALJON, S. WILLIAMS, San Diego State University, N. BALABAEV, Institute of Mathematical Problems of Biology, Pushchino, Russia, F. PAANS, A. LYULIN, Dutch Polymer Institute, Technical University Eindhoven, The Netherlands — By means of large-scale computer simulations we investigate relaxation processes in polystyrene melts and ultra-thin films. The local orientational mobility of the phenyl bonds is studied with the help of Legendre polynomials of the second-order  $P_2(t)$ . The spectral density of  $P_2(t)$  shows several distinctive peaks. They are caused by the large-scale motions of cooperative segments ( $\alpha$  relaxation), smaller-scale structural dynamics ( $\beta$  relaxation), and transient processes. Our simulations reveal that interfaces affect  $\alpha$ - and  $\beta$ -relaxation processes differently. The most puzzling observation is a slight decrease in the structural relaxation time in the middle of the film, compared to that near the free surface. As expected, the  $\alpha$ -relaxation time is shorter near the free surface. The glass transition temperature, obtained from a plot of thickness versus temperature, decreases with decreasing film thickness, which is in agreement with an observed decrease in the  $\alpha$ -relaxation time. Surprisingly, the structural relaxation time is roughly the same for the bulk and for films. Our results will be compared with published experimental data.

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