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### **Confinement effects on polymer structure and glassy dynamics<sup>1</sup>**

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We have performed molecular-dynamics simulations to explore the influence of confinement on the glass-transition temperature  $T_g$  for supported atactic-polystyrene thin films of different thickness (1 nm ÷ 10 nm) and different strengths of attraction to the substrate (0.1 kcal/mol ÷ 3.0 kcal/mol). The films have been equilibrated in a melt at 540 K and further cooled down with a constant cooling velocity of 0.01 K/ps below  $T_g$  to room temperature, 300 K. Based on the density measurements we have defined three different (substrate, middle and surface) layers for each film. We found that the monomers close to the surface and in the substrate layer are partially oriented, which leads to more effective monomer packing. For the whole film the average  $T_g$  value remains almost constant for films down to 2 nm thickness, where middle layer vanishes. For the middle layer itself  $T_g$  does not depend on the total film thickness, while an increase up to 70 K is measured for the substrate layer depending on the strength of attraction to the actual substrate. The surface layer remains liquid-like in the whole temperature range (300 K ÷ 540 K). We claim that the redistribution of mass in the three film layers may explain the change with film thickness of the average  $T_g$ , if the latter is determined from linear fits of the average glass and melt densities. First results on the shear cycling and the rejuvenation phenomena will be discussed as well.

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