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Substrate effects on the relaxation dynamics of nano-confined polymers: Insight from MD simulations[1]

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In this talk, I survey recent progress in understanding the structure and dynamics of ultra thin polymer melts confined between solid walls. Here, “ultra” refers to distances between the substrates of the order of a few radius of gyration of the polymer chain. Using the example of a coarse-grained polymer model, we explore in detail the influence of the boundary condition, imposed by smooth or rough walls, on the structure and dynamics of the polymer melt. Depending on the atomic structure of the substrate, geometric confinement is found to have quite opposite effects on the properties of the melt. While polymers diffuse faster compared to the bulk in the vicinity of a perfectly smooth wall (no corrugation at all), their dynamics is strongly hampered close to a wall exhibiting corrugation on the length scale of the monomer diameter. The effect of corrugation is further enhanced if the wall atoms are not distributed randomly but are placed on a crystalline lattice. These effects are by no means negligible since they can change the structural relaxation time by many orders of magnitude. As a consequence, in nano-confined polymer systems, the glass transition temperature is expected to significantly differ from its bulk value. We compare our and other simulation results with experimental data and survey some theoretical ideas to explain these shifts.

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