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Polymer Melts inside Nanoscale Cylindrical Pores: Chain Conformations, Polymer Diffusion and Local Dynamics

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ABSTRACT

Polymers in composites and inside porous media are frequently confined to spaces that are comparable to or even smaller than their mean end-to-end distances in the unconfined bulk state. Understanding the impact of nanoscale confinement on both polymer structure and dynamics is critical for a variety of applications including hydraulic fracturing fluids, porous inorganic thin films in the electronics industry, and composites. To date, our work focuses on polymer melts under nanoscale cylindrical confinement. The polymer center-of-mass diffusion into cylindrical pores in anodized aluminum oxide membranes (diameters 18 – 80 nm) was measured using elastic recoil detection. This ion beam method that provides the concentration profile of deuterated polystyrene (400 kg/mol) penetrating into the AAO membranes prefilled with polystyrene (200 or 290 kg/mol). The polymer diffusion coefficient increases with decreasing pore diameter. This experimental finding is corroborated by coarse grain simulations with neutral interactions with the pore walls, although the increase is more pronounced in the simulations. The simulations previously found that chain conformations slightly elongated parallel to the cylinder axis and compressed perpendicular to the cylinder and the number of entanglements per chain decreases as the cylinder diameter decreases. It is primarily the reduction in polymer entanglements that allows polymers to diffuse faster when the pore diameter is smaller. We have also probed the local polymer dynamics using quasi-elastic neutron scattering.