

Abstract Submitted
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Polymer Structure and Dynamics under Cylindrical Confinement: Experiments, Simulations and Theory¹ WEI-SHAO TUNG, DANIEL SUSSMAN, University of Pennsylvania, NIGEL CLARKE, University of Sheffield, RUSSELL COMPOSTO, University of Pennsylvania, KENNETH SCHWEIZER, University of Illinois, ROBERT RIGGLEMAN, KAREN WINEY, University of Pennsylvania — Polymer structure and dynamics are perturbed under confinement, especially when the dimension of the confinement is smaller than the polymer's radius of gyration (R_g). While most studies focus on thin film confinement, we study cylindrical confinement using experiments, simulations and theory. Our MD simulations study the change in R_g , local dynamics, entanglement molecular weight (N_e), and diffusion coefficient (D) for polymers in cylindrical confinement with different diameters ($d/2R_g \sim 0.4 - 6$). We found increased N_e and D in cylindrical confinement for $d/2R_g < 1.5$. Moreover, R_g decreases in the direction of confinement and increases along the cylinder axis. We developed an analytical theory to relate the transformation of chain conformations to the preferential orientation of primitive path steps, and further predicted the increase of N_e . Experimentally, we infiltrated 400 kg/mol polystyrene ($2R_g \sim 35\text{nm}$) into anodized aluminum oxide (AAO) membranes ($d \sim 18\text{-}150\text{nm}$) to confine polymers into cylindrical nanopores ($d/R_g \sim 0.5\text{-}4$). We use SANS to probe R_g , QENS to probe the local dynamics, and elastic recoil detection to measure D of deuterated PS inside PS-filled AAO nanopores. Values obtained from our experiments and literature are quantitatively compared with our simulation results.

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