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Structure and Dynamics of Polymers in Cylindrical Nanoconfinement: A Molecular Dynamics Study JAMES PRESSLY, ROBERT RIGGLEMAN, KAREN WINEY, Univ of Pennsylvania — The structure and dynamics of polymers under nanoconfinement is critical for understanding how polymers behave in applications from hydraulic fracking to fabricating integrated circuits. We previously used simulations to explore the effect of the diameter of cylindrical pores ($d = 10-40\sigma$, where σ is the unit length in reduced units) on polymer end-to-end distance ($R_{ee,perp}$, $R_{ee,par}$), entanglement density, melt diffusion coefficient (D), and local relaxation time (τ_{perp} , τ_{par}) at fixed polymer chain length ($N = 350$). These studies found D , $R_{ee,par}$, and τ_{perp} increased with increasing confinement while entanglement density, $R_{ee,perp}$, and τ_{par} decreased. Experiments also found that D increased but to a lesser extent. Here, we examine the molecular weight dependence of these properties using $N = 25, 50, 100, 200, 350$, and 500 confined to pores of diameter 14σ to examine a range of confinements. Our preliminary results show that as N increases D and $R_{ee,par}$ increase as well, relative to the unconfined state, while entanglement density and $R_{ee,perp}$ decrease, consistent with our previous work. Interestingly, τ is shown to be independent of chain length indicating the impact of confinement imposed by reducing pore diameter is distinct from that imposed by increasing chain length.

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