172d A Monte Carlo Study of Chain Conformation in a Cylindrical Confinement

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Off-lattice Monte Carlo simulations are applied to study the behavior of chain molecules confined in a long cylindrical pore under the condition of hard-body interaction. The emphasis is placed on the chain and bead distributions as well as the location dependence of the chain conformation and anisotropy. The simulation results show that the chains very near the pore surface tend to wrap around the surface in various configurations. This behavior is qualitatively analogous to that of chains near but outside a cylindrical rod. Moreover, the bead concentration near the pore surface increases with increasing surface curvature.