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Tube Visualization and Properties from Isoconfigurational Averaging JIAN QIN, WINDSOR BISBEE, SCOTT MILNER, Dept. of Ch. E. at Penn. State Univ. — We introduce a simulation method to visualize the confining tube in polymer melts and measure its properties. We studied bead-spring ring polymers, which conveniently suppresses constraint release and contour length fluctuations. We allow molecules to cross and reach topologically equilibrated states by invoking various molecular rebridging moves in Monte Carlo simulations. To reveal the confining tube, we start with a well equilibrated configuration, turn off rebridging moves, and run molecular dynamics simulation multiple times, each with different initial velocities. The resulting set of "movies" of molecular trajectories defines an isoconfigurational ensemble, with the bead positions at different times and in different "movies" giving rise to a cloud. The cloud shows the shape, range and strength of the tube confinement, which enables us to study the statistical properties of tube. Using this approach, we studied the effects of free surface, and found that the tube diameter near the surface is greater than the bulk value by about 25%.

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