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Multiphase Transitions Involving Confined Polymers in Solution

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There has been a growing interest in the study of deformation of a nanochannel confined polymer as it plays an important role in biological phenomena such as DNA mapping, DNA condensation, protein folding, and chromatin organization. Therefore, it is important to investigate the statistics and dynamics of confined polymers and predict their time and space evolution. Acquiring information on polymer concentration can be used to model transient and steady-state non-equilibrium phenomena such as compression against defects and chain stretching and compression in crossing the region of low to high confinement. In our work, we studied the compression of a long polymer chain with 256 monomers confined in a nanochannel by being pushed in a fluid by a large sphere through the channel. We used LBMD(lattice-Boltzmann molecular dynamics) to model the particles and the fluid in the channel. We used a wide range of sphere speeds and investigated how the sphere's speed affects the configuration of a confined chain in a nanochannel. At different chain speeds, different states of compaction of the polymer are observed. At intermediate speeds, these states can coexist. We characterize and map out a phase diagram of these states.

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