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Dynamics of chain stiffening of a semiflexible bead-rod polymer

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Abstract

This talk considers the dynamics of chain stiffening of a semiflexible bead-rod polymer in a viscous solvent. Examples of semiflexible polymers include biopolymers such as DNA, actin filaments microtubules, MTV and other viruses. Physically this problem may correspond to the case of a polymer chain stiffening due to addition of a solute or a change in the temperature.

Methodology

To study this problem, Brownian Dynamics simulations based on a discretized version of the worm-like model are employed over a broad range of time scales and polymer lengths. The configuration, stress and tension evolution are presented over extended time periods.

Conclusions

In this talk we discuss the associated coil-to-helix-to-rod transition. To determine the evolution mechanism of the polymer chain we utilize the methodologies we have developed in our previous studies (J. Chem. Phys. 119, 2003; Phys. Rev. Lett. 93, 2004). In particular, the chain evolution is determined over extended time periods by monitoring the eigenvalues of the chain's gyration tensor while the forces along the polymer chains are determined numerically over the same extended time periods.