Canadian Association of Physicists | Association canadienne des physiciens et physiciennes

Contribution ID: **1636** Type: **not specified**

Simulation study of overlapping polymers under confinement

Sunday, 28 May 2017 09:30 (15 minutes)

Polymers subject to confinement in a narrow channel tend to be linearly ordered along the axis of the channel. When such a confined polymer is in a folded state, the internal overlap leads to a reduction in conformational entropy that increases the free energy. A similar effect arises when two different polymers overlap along the channel. In each case, the free energy tends to increase with increasing overlap, giving rise to entropic forces that drive unfolding or chain segregation. In this study, Monte Carlo simulations are used to measure the free energy of polymers subject to cylindrical confinement. The calculated free energy functions are used to test the predictions of scaling theories and quantify the finite-size effects. We focus on the effects of bending rigidity and macromolecular crowding. For a single-polymer system, we calculate the free energy as a function of extension length for a wormlike chain in the Odijk regime in cases where there is either one or two folds in the chain. The results are generally in agreement with the predictions of simple scaling arguments, though quantitative discrepancies persist for chains up to 400 monomers in length due to finite-size effects. We also measure the free energy functions for a system of two flexible polymers in the presence of mobile crowding agents. We find that increasing crowder packing fraction tends to decrease the overlap free energy cost. However, for fixed packing fraction, the free energy barrier increases as the crowder/monomer size ratio decreases. The relevance of these results to the process of chromosome segregation in replicating bacteria is discussed.

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Session Classification: Soft Matter Canada 2017 / Matière molle Canada 2017

Track Classification: Soft Matter Canada 2017