SUMMARY OF Ph.D. DISSERTATION

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Title

Effects of Topological Constraints of Knots on Single Ring Polymers

Abstract

A single knotted ring polymer is one of the self-entangled systems and can be considered as an ideal system for the study of topological effects. The purpose of this study is to examine the effects of topological constraints on the properties of single knotted ring polymers. The relaxation, the average structures and the knotted part of a ring polymer with the trefoil knot are studied through Brownian dynamics simulations of a bead-spring model of a ring polymer with N segments in good solvent.

In chapter 1, we give a general introduction for the present thesis. Chapters 2, 3 and 4 are devoted to the descriptions of knot theory, polymer physics and simulations.

In chapter 4, the effects of the topological constraints on the relaxation are examined. The relaxation rate for the wave number q is estimated from the time correlation function of the Fourier transform of the segment positions. The wave number of the slowest relaxation rate for each N changes from $q = 2$ to $q = 1$ around $N_c = 96$~144 as N increases. This transition is considered to correspond to the knot localization, where the knotted part becomes localized to a part of the polymer as N increases.

In chapter 5, the knot localization is studied by directly observing its average structure in three dimensions through simulations. The average structure is self-consistently defined as the average of conformation vectors obtained from a simulation each of which is translated and rotated to minimize its distance form the average of the conformation vectors. An extension of the definition of the average structure is proposed by utilizing the symmetry of a homopolymer. The knotted part of each average structure is delocalized below $N_x = 120$ and becomes localized as N increases.

In chapter 6, the N-dependence of the length of a knotted partial chain is examined by applying the new definition of the knotted partial chain. The knotted partial chain is defined as the shortest partial chain, which has the same knot-type as that of the original polymer when its ends are connected each other by the path on the sphere separating the partial chain and the rest of the ring polymer spatially. The equilibrium average of the length of knotted partial chain shows the power law behavior $\langle \ell_K \rangle \propto N^t$, $t \simeq 0.8$. The value of t suggests the knot localization since $t < 1$.

Finally, we conclude that these studies provide strong evidence for the knot localization.