Intrinsic viscosity of knots in solution evaluated through the Brownian Dynamics

Naoko Kanaeda[1] and Tetsuo Deguchi[2], Department of Physics,
Graduate School of Humanities and Sciences, Ochanomizu University,
Ohtsuka 2-1-1, Bunkyo-ku, Tokyo 112-8610 Japan

Abstract: We have evaluated the intrinsic viscosity of the solution of ring polymers of a knot type K by the Brownian dynamics with both hydrodynamic and excluded volume effects. Due to recent development of experiments, we expect that knotted ring polymers will be synthesized near future. It is thus important to formulate empirical equations for describing the intrinsic viscosity in terms of K. They should be useful for separating knot species in solution. We found that the ratio of the intrinsic viscosity of a knot to that of the trefoil knot is independent of the number of segments N in the investigated range. We also found that it is expressed by a quadratic function of the average crossing number of the ideal knot of K (ACN(K)).

我々は溶液中における結び目高分子の固有粘度を、Brownian dynamics により排除体積効果および流体力学的相互作用を考慮して計算した。近年の実験技術の進展により、結び目高分子の合成が予見される中で、溶液の固有粘度を表す公式を導入することは重要である。また結び目高分子は溶液中に混在しているため、それらの分離にも役立つことが期待される。その結果、結び目高分子の三葉結び目に対する固有粘度の比が、N に依存しないことが分かった。またその固有粘度の比は、理想結び目の平均交点数(ACN)の二次関数であることも分かった。

1. Introduction

In this work, we have investigated the intrinsic viscosity of the solution of knotted ring-polymers through the Brownian dynamics with hydrodynamic and excluded volume effects. In recent experiments, ring polymers of high purity have been synthesized with small dispersion [1]. We thus expect that knotted ring polymers will be synthesized near future. It is then important to express the intrinsic viscosity of the solution of knotted ring polymers with the same knot type K in terms of knot K. We formulate an empirical equation of the ratio of the intrinsic viscosity of a nontrivial knot to that of the trefoil knot expressed in terms of the average crossing number of ideal knot of knot K (ACN(K)). Here we remark that the ideal knot should play a fundamental role in the dynamics of knots in solution. In fact we have found in the previous study that the ratio of the diffusion constant of a nontrivial knot to that of a linear polymer is almost independent of the number of segments N, and also that it is given by a linear function of ACN(K) [2].

2. Result

Fig. 1 shows the N-dependence of the intrinsic viscosity $[\eta]/[\eta]_0$ for the trefoil knot in the case of N=20, 27 and 36 (here $[\eta]_0$ is the zero-shear viscosity for the Rouse model). The intrinsic viscosity at shear rate γ depends on the number of segments N. However, in Fig. 2 we find that the intrinsic viscosity divided by $N^{0.8}$ is independent of N. For other knots such as the 4_1 knot and the 5_1 knot, the intrinsic viscosity divided by $N^{0.8}$ is almost independent of N. In our numerical simulation, we have $[\eta]_K=a(K)\,[\eta]_0 N^{0.8}$ for any given knot type K, where the coefficient a(K) depends on the shear rate γ. Therefore, the ratio of the intrinsic viscosity of a nontrivial knot to that of the trefoil knot is given by $[\eta]_K/[\eta]_{31}=a(K)/a(3_1)$.

Fig 1.

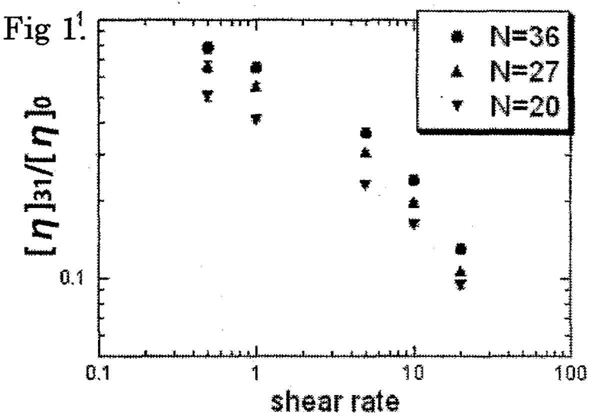
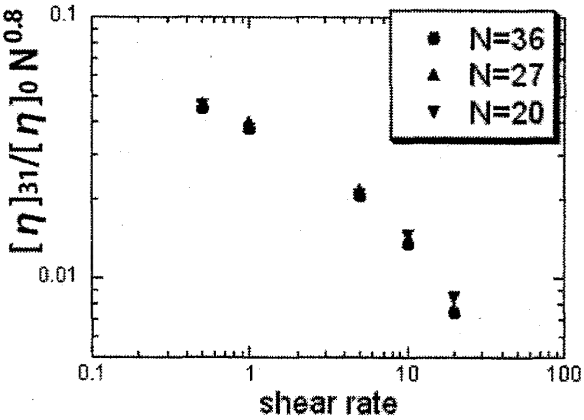


Fig2



We have found that the ratio $[\eta]_K/[\eta]_{31}$ is expressed as a quadratic function of ACN(N) and shear rate γ. In the case of high shear rate, we have

$$[\eta]_K/[\eta]_{31}$$

$$=-0.00045\gamma((ACN(K)-ACN(3_1))^2+460\gamma^{-2}(ACN(K)-ACN(3_1)))+1.0$$

In the case of low shear rate, we have

$$[\eta]_K/[\eta]_{31}$$

$$=0.0028\gamma^{-1}((ACN(K)-ACN(3_1))^2-37\gamma(ACN(K)-ACN(3_1)))+1.0$$

These empirical equations should be independent of N in the investigated range.

3. Conclusion

The ratio of intrinsic viscosities $[\eta]_K/[\eta]_{31}$ is almost independent of N. This ratio is expressed as the quadratic function of ACN(K). Furthermore we suggest that the ideal knot should be a fundamental concept in the dynamics of knots in solution.

References

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1 kanaeda@degway.phys.ocha.ac.jp 2 deguchi@phys.ocha.ac.jp