

# Self-Organized Structures of a Single Polymer Chain

## — Morphological Variation of Toroids —

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単一セミフレキシブル高分子は、貧溶媒環境下においてランダムコイル状態からグロビュール状態への一次相転移を起こし、自発的に様々な形状に折り畳まれる。本研究では、特にセミフレキシブル鎖の凝縮状態によく見られるトロイド構造に着目して、高分子鎖の太さ、硬さ、荷電といった物性と、折り畳み後の形状との関係を解析的に明らかにする。

### 1 Introduction

Among polymers, particularly interesting is a semiflexible polymer, such as a giant DNA, for which the inequality  $\delta \ll \lambda \ll L$  is satisfied, where  $\delta$ ,  $\lambda$  and  $L$  is thickness, persistence length and contour length of a chain respectively. Indeed, with a decrease in the solvent quality or in the presence of condensing agents, the single chain undergoes a first-order phase transition between an elongated coil and a very dense, compact states[1]. As the result of folding transition, the compact chains can spontaneously show various morphologies.

In this study, we have investigated the morphologies of a single polymer chain after the folding transition by using a simple theoretical approach. We will start from the situation of a neutral chain and next the electrostatic effect will be taken into account.

### 2 Results

We assume the toroidal cross section  $(x, y)$  as the multiple of a line and a semicircle. Based on this model, we calculate the total energy  $F_{neutral}$  under such condition that the contour length is constant  $L$ . For calculating  $F_{neutral}$ , we consider only the bending energy and the surface energy for simplicity.

$$F_{neutral} = F_b + F_s = \frac{4\pi P}{d} \int_{R-r}^{R+r} \frac{y}{x} dx + 4\pi\sigma X_0 \int_{R-r}^{R+r} \left\{1 + \left(\frac{dy}{dx}\right)^2\right\}^{\frac{1}{2}} dx, \quad (1)$$

where  $\sigma$  and  $X_0$  is the surface tension of a toroid and the x-coordinate of the center of mass of a cross section respectively. By minimizing the total energy  $F_{neutral}$  with respect to toroidal parameters,  $R$ ,  $r$  and  $c$ , we can obtain the optimum dimension of a toroid. Fig. 1 (a) shows the effects of stiffness and thickness of a chain on the toroidal morphology[2].

When we take the electrostatic effect into account, the situation is much different. We consider a simple theoretical approach of the condensed states made of a single charged chain with a fixed charge density.

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The total free energy of multi-tori made of  $n$  toroids can be expressed[3] as

$$F_{charge} = (-ar^3 + br^2 + c\frac{q^2}{r})n \sim -aV + bV^{\frac{2}{3}}n^{\frac{1}{3}} + cV^{\frac{5}{3}}n^{-\frac{2}{3}}, \quad (2)$$

where  $r$  is the average radius and  $q$  is the remaining charge on each condensate and  $V$  is the volume of multi-tori, which is proportional to the contour length of a chain, and  $a$ ,  $b$ , and  $c$  are positive constants. By minimizing the free energy  $F_{charge}$ , we can obtain the relationship between contour length and the number of compact states  $n$  as shown in Fig. 1 (b).

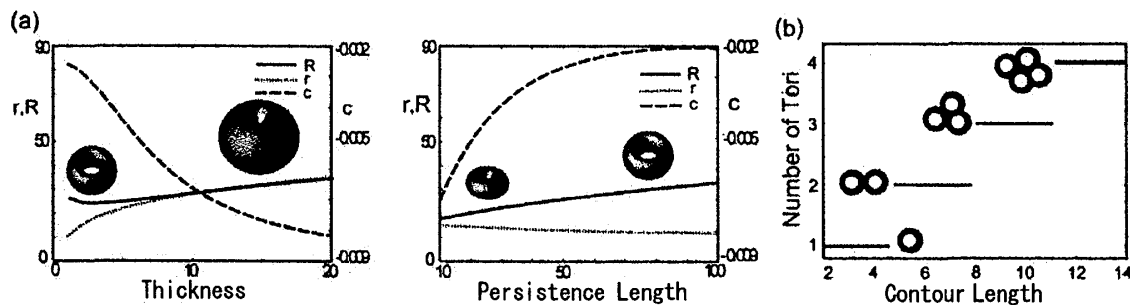


Figure 1: Results of theoretical calculations. (a) Morphological changes on toroid as a function of thickness and stiffness of a chain. Giant toroid can be appeared by choosing proper parameters.  $R$ ,  $r$  and  $c$  is the average radius, the thickness of a toroid without deformation and the parameter of deformation of a toroid respectively. In the graphs, the characteristic toroids are shown. (b) Number of tori as a function of the contour length, as the self-organized structure from a single polyelectrolyte. Each horizontal bar indicates the region where a given morphology is the most stable. It shows that the number of tori increases with an increase in contour length because of the instability due to the remaining charge on each condensate.

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