

# Core-shell structure in semiflexible-flexible block copolymers

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本研究では、異なる曲げ弾性率を持つブロック共重合体の折り畳み相転移について議論する。シミュレーションを行った結果、“柔らかい”ブロックが核を形成し、その周りに“硬い”ブロックが巻きつくといった、いわゆるコア-シェル状の折りたたみ構造を持つことが明らかになった。この構造は、一様な曲げ弾性率を持つ高分子(セミフレキシブル高分子)と比べて二つの点で異なっている。一つは、一様な高分子の場合と比べて非常に効率的に折り畳まれるという点であり、二つ目は、折り畳みの経路に依存しないという点である。後者については、一様高分子の折り畳み構造の一つである筒状構造の不安定化によって議論することができる。

## 1 Introduction

Polymer-based nanostructures have been extensively studied due to their importance in industrial applications, particularly in nanodevices and nanomachines. They are also of importance in living cells; DNA and protein molecules have nano-ordered structures, which show a close relationship with their biological functions. Macromolecules in biological systems typically undergo conformational transitions. Since a lot of macromolecules, particularly biomacromolecules, have ordered, folded structures, there has recently been much attention to semiflexible homopolymers, which show bending rigidity along the chain, and, as a result, have a rod-like properties, although their contour lengths are long enough to exhibit overall fluctuations. A semiflexible homopolymer has been extensively studied as a model for a DNA molecules. In living systems, however, biopolymers such as proteins are, in general, heteropolymers with complicated sequences of amino acids. Since our understanding of role of heterogeneity in bending rigidity is still primitive, in this presentation, we propose a minimum model to extend the concept of semiflexible polymers toward heteropolymers. A single block copolymer is the simplest extension of a single homopolymer in the direction of single heteropolymers such as proteins. To this end, we concentrate on a simple model: diblock copolymers in which two blocks possess different levels of flexibility.

## 2 Core-shell structure and folding kinetics

We carried out Langevin dynamics simulations to explore conformation of the rod-coil block copolymer at folded state. Our results show that the final conformation of the rod-coil copolymer is the uniquely

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determined core-shell structure, in which the flexible block at the core is surrounded by the semiflexible block (Fig.1C(e)).

We show in Fig. 1 the kinetics of the formation for the core-shell structure, where we suddenly increase the attractive interaction between monomers  $\epsilon$  at  $t = 0$ . The flexible block collapses at an early stage, and the semiflexible block then gradually wraps around it. This is contrast to the situation for flexible and semiflexible homopolymers: flexible polymers exhibit spinodal decomposition in the folding process, whereas semiflexible polymers undergo a nucleation and coarsening process. Due to a stochastic feature of nucleation, there is a long lag time before the folding transition in a semiflexible polymer takes place. These observations indicates that the rod-coil copolymer collapses much more quickly than a semiflexible polymer. Figure 1 shows the time evolution in the collapse ratio. As we can see, rod-coil copolymers undergo folding more quickly than semiflexible homopolymers.

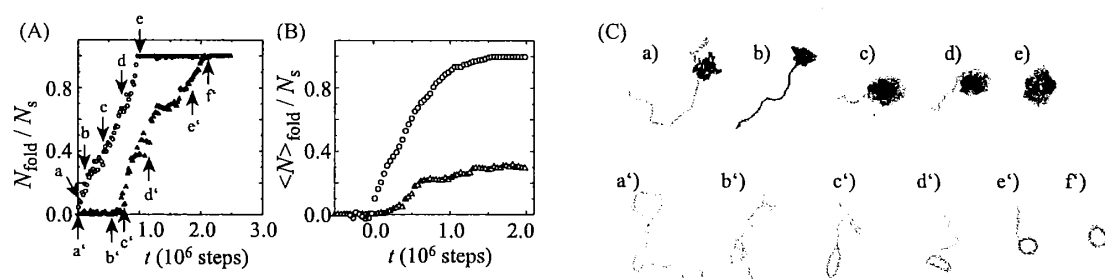


Figure 1: Time evolution of the number of collapsed monomers in the semiflexible block of a rod-coil copolymer (○) and a semiflexible homopolymer (△). Each polymer has  $N = 256$  monomers, and a bending elasticity  $\kappa_s = 15$  for the semiflexible parts. We change the attractive interaction at  $t = 0$  to  $\epsilon = 0.8$ .  $N_{\text{fold}}$  shows the number of monomers in the folded state. The bare data are shown in (A), while the mean evolution over 30 runs is shown in (B). Snapshots of the polymer conformation during the transition for a rod-coil copolymer (a-f) and a semiflexible homopolymer (a'-f') are shown in (C).

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## References

- [1] N. Yoshinaga and K. Yoshikawa, J. Chem. Phys. in press (arXiv:0706.1389).