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Tensile Tests of DNA by Steered Molecular Dynamics

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Summary

Self-assembled DNA network on a substrate will play a key role in the fabrication process of bio-nano devices. Figure 1 shows the AFM image of 50 bp poly(dA)·poly(dT) DNA network on a mica surface. It can be observed that three branches of the DNA network join together at each junction. Characteristics of such network structure depend on the mechanical properties of the constituent DNA molecules, but they are not fully accessible from the experiments.

Therefore, we have conducted steered molecular dynamics (SMD) simulation of 10-bp poly(dA)·poly(dT) DNA in order to clarify the tensile properties. Figure 2 shows the force F as a function of the end-to-end distance x obtained from our simulation and previous experimental results by Smith et al. (*Science*, Vol. 271, pp. 795-799 (1996)), where x is normalized by the contour length of 3.4 nm. The entropic elasticity is negligible in the present study since the DNA used here is much shorter than its persistence length $P \cong 50$ nm. In the process of tensile test, structural transition from B-DNA to ladder-like S-DNA is observed in the domain of $1.0 < x < 1.7$. The magnitude of the force is smaller than the experimental result there, which is attributed to the absence of the counter ions in the simulation. Nevertheless, the numerical result precisely predicts the drastic increase of the force at around $x = 1.7$. The SMD not only reproduces the previous experimental results but also reveals the elementary process of structural transition in a molecule.

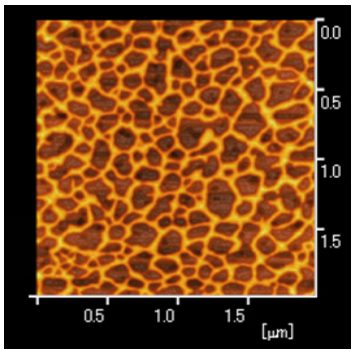

Figure 1: AFM image of the self-assembled DNA network structure

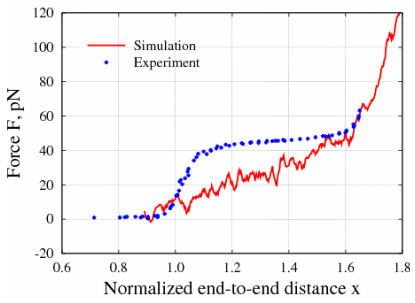

Figure 2: Force-extension curves obtained from our present study and that from previous experiment by S. B. Smith et al.

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