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Recorrection Stretch Function Of the Spring-Like Elastic DNA Molecules

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Abstract - In many works, the stretch function to describe the dependence of the elastic force on the extension is derived experimentally or using the Newton interpolation formula. The stretching functions in previous approach are usefull for the large value, but not small value of extension. Especially, they are not true when the extension equal to the stable length, at which the elastic force must be ignored and to the contour length, at which elastic force must be finite. From above evaluations, in this paper we present the analyzing the experimental data and deriving the corrected stretching functions for the spring-like elastic DNA molecules. Based on the experimental elastic parameters the recorrected stretch function is simulated to confirm its accuracy comparable to experimental F-x characteristic. The results should be useful for simulation the operation of optical tweezer for biological systems.

Index Terms **- Optical tweezer, DNA molecules, Elastic force, Extension, Worm –like chain.**

I. INTRODUCTION

There are many interests in optical trap to investigate bio-molecules, especially, DNA molecules [1]-[10]. The main purposes are investigation the nanomechanics, elastic force, spring contant, etc. of DNA molecules. The obtained results are focused on the elastic parameters, which give to express experimentally [1], approximately [2], [3] or using Newton interpolation formula [4] the stretch function describing dependence of the elastic force on extension of DNA molecules. Unfortunately, the approximation stretch function given by Bustamante [2], Baumann [3] and Mack [6] can not be used to simulated the dynamic of DNA molecules in an optical trap [11], [12], because of that by using this function the elastic force at the contour length (maximum length of DNA) is infinity, which is more larger than reachable optical force. In this paper we recorrect the approximation stretch function and discuss its accuracy based on the experimental elastic parameters.

II. ELASTIC FORCE ON PREVIOUS APPROACH

The entropy spring-like forces of DNA molecule can be understood by a worm-like chain (WLC) model as shown in Fig.1 [1]. One DNA molecule consists of n segments, which has length l, and has a stable length $L_{st} = nl$ and contour length L (or maximum length) [1].

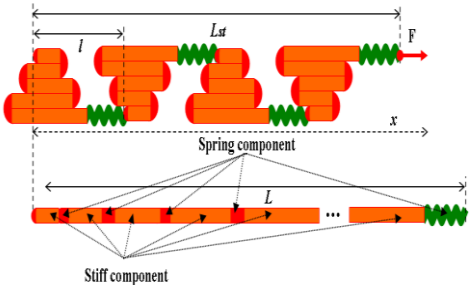

Fig.1 WLC model of fibrillin molecule.

The elastic force, F is approximately given as following [1], [2], [3] and [13]

$$F(x) = \frac{k_B T}{L_{st}}\left[\frac{x}{L} + \frac{1}{4}\frac{1}{(1-x/L)^2} - \frac{1}{4}\right] \quad (1)$$

where x is the extension (end-to-end length) (m), $k_B = 1.381\times10^{-23}\,J/K$ is the Boltzmann constant, T is the absolute temperature (K), L_{st} is the stable length without stretching (m), L is the contour length-the maximum length (m). A modification of Eq.1 that takes into account stretching of the DNA at or slightly beyond full extension is approximately given by [3], [6]:

$$\frac{F(x)L_{st}}{k_b T} = \frac{1}{4}\left(1 - \frac{x}{L} + \frac{F(x)}{K_0}\right)^2 + \frac{x}{L} - \frac{1}{4} - \frac{F(x)}{K_0} \quad (2)$$

Where K_0 is the stretch modulus?

Table 1. Measured DNA elastic parameters with various ionic conditions.

Sample Number	Buffer composition	L_{st} (nm)	K_0 (pN)	L (nm)
	Plasmid DNA			
1.	10mM Na^+	47.4 ± 1.0 (10)	1008 ± 38 (10)	1343 ± 5(10)
2.	10mM Na^+ và 10μM Spd^{3+}	40.7 ± 1.4 (11)	1166 ± 114 (6)	1353 ± 5(6)
3.	10mM Na^+ và 100μM Spd^{3+}	38.7 ± 1.0 (8)	1202 ± 83 (5)	1313 ± 2(5)
4.	10mM Na^+ và 200μM Spd^{3+}	40.6 ± 1.1 (8)	1253 ± 158 (2)	1318 ± 12(3)
5.	10mM Na^+ và 300μM Spd^{3+}	38.9 ± 0.8 (2)	1070 ± 158 (2)	1333 ± 11(2)
	λ DNA			
6.	9.3mM Na^+ và 100μM CoHex	44.7		16,674
7.	186mM Na^+ và 100μM Spd^{3+}	48.0		16,621
8.	186mM Na^+	54.1 ± 3.3 (3)		16,745 ± 82.4 (3)
9.	1.86mM Na^+ và 100μM CoHex	32.4 ± 1.4 (3)		16,742
10.	1.86mM Na^+	86.2 ± 4.9 (7)		16,748 ± 76 (7)

Spd^{3+} : spermidine; (number of molecules)

Using the experimentally measured elastic parameters in Tab.1 [3], the dependence of the elastic force F on the extension, x for some DNA molecules can be derived by resolution the quadratic equation given as following [4]:

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$$16A^2 f^2 + \left[8A(1-4y)+1\right] f + y(16y+7) = 0 \quad (3)$$

where $A = 1 + K_0 L_b / k_B T$ $f = F / K_0$ $y = x / L$ or using Newton interpolation formula as [4]:

$$f(x) \approx 0{,}556x^3 - 20{,}545x^2 + 251{,}155x - 1013{,}765 \quad (4)$$

for λ DNA sample No.7 in Tab.1.

Unfortunately, for some DNA molecules some of elastic parameters are unknown or not be experimentally measured, so the dependence of the elastic force on the extension are given by the experimental F-x characteristics, which are illustrated in Fig.2 [3], [13].

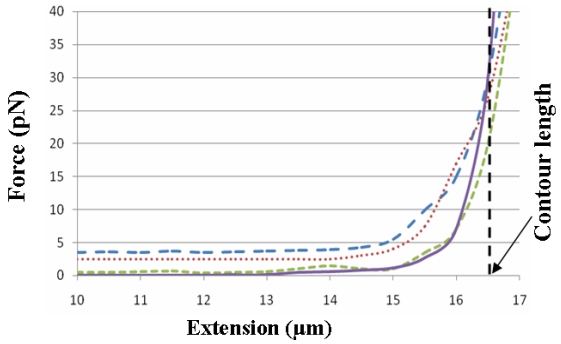

Fig.2 Response of single λ DNA molecules to an applied force with condensing concentrations of trivalent cations CoHex and Spermidine: WLC with L_{st}=95nm and L=16500nm (Gyan-solid); Sample No. 6 (Green-dash); No. 8 (Blue-long dash); No. 10 (Red-dots curve) [3].

Carefully investigating all stretch functions given in previous approach [1], [2], [3], [6], [13], there are following questions to discuss:

From Eq. 1:

1) Because $x < L$, so that the elastic force increases with increasing of extension, that is real and can be accepted;

2) $F = 0$ when x=0, but $F \neq 0$ when $x = L_{st}$, this is not real and can not be accepted (this comment will be similar to Eq.2 and Eq. 4);

3) if $x \to L$ means $1 - x/L \to 0$ and then $F \to \infty$, this is not real, because $F(L) \gg K_0$ (see Fig.2 and Tab.1) and can not be accepted.

Eq. 2, can be rewritten as:

$$\frac{FL_{st}}{k_b T} = \frac{x}{L}\left[1 - \frac{1}{2}\left(1 - \frac{F}{K_0}\right)\right] + \frac{1}{4}\left(\frac{x}{L}\right)^2 - \frac{3}{2}\frac{F}{K_0} + \frac{1}{4}\left(\frac{F}{K_0}\right)^2 \quad (5)$$

$$\approx \frac{1}{2}\frac{x}{L} + \frac{1}{4}\left(\frac{x}{L}\right)^2 \quad if\ F \ll K_0$$

and give us some attention points:

4) Because $F \ll K_0$ (see Tab.1 and Fig.2), so that elastic force is proportional to extension, this is real and accepted;

From the nature structure of the DNA molecules and the their spring-like chain as shown in Fig.1, following proposed points will be clear to pay attention:

i) The extension, x is never equal zero (always $x \neq 0$), but always shorter than the contour length ($x < L$) and longer than the stable length ($x \geq L_{st}$);

ii) The elastic force is always positive ($F(x) > 0$) at stretching state (when $x > L_{st}$), smaller than the stretching limit ($F(L) < F_{\lim}$) and will be ignored ($F(L_{st}) = 0$) at relaxation state of DNA ($x = L_{st}$);

iii) If $x > L$ the DNA molecule is at irreversible state, means the spring constant is to be zero, consequently, the limit (or maximum) elastic force is comparable to stretch modulus ($F_{\lim} \leq K_0$) only.

To describe the nature of spring-like chain of DNA molecules as well as above proposed points, the stretching functions should be modified or recorrected.

III. RECORRECTION STRETCH FUNCTION

From equation (1), the elastic force at stable length will be zero, if following equation satisfies:

$$\left[\frac{L_{st}}{L} + \frac{1}{4}\frac{1}{\left(1 - L_{st}/L\right)^2} - \frac{1}{4}\right] = 0 \quad (6)$$

But for a DNA molecule, the contour length and the stable length are constant, so following relations must be satisfied:

$$\frac{L_{st}}{L} \neq 0 \text{ and } \frac{1}{4}\frac{1}{\left(1 - L_{st}/L\right)^2} - \frac{1}{4} \neq 0 \quad (7)$$

From Eq.6, two relations in Eq.7 will be equation at stable length (as shown in point ii) if L_{st}/L is replaced by $\left(L_{st} - L_{st}\right)/L$ only. That means, the term x/L must be replaced by $\left(x - L_{st}\right)/L$ in Eq.1. With experimentally measured elastic parameters as shown in Tab.1, $L_{st} \gg L$ [2], [5], so $\left(x - L_{st}\right)/L = x/L - L_{st}/L \approx x/L$ and Eq.1 can be slightly modified as:

$$F(x) = \frac{k_B T}{L_{st}}\left[\frac{x - L_{st}}{L} + \frac{1}{4}\frac{1}{\left[1 - \left(x - L_{st}\right)/L\right]^2} - \frac{1}{4}\right] \quad (8)$$

The recorrected stretch function in Eq.8 satisfies reality of spring-like chain of DNA molecules as shown above, in detail,

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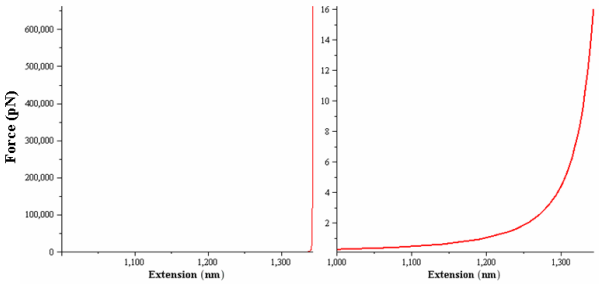
$$F(x)=\begin{cases} i)\ \ F(L_{st})>0 & if\ \ x>L_{st}, \\ ii)\ \ 0 & if\ \ x=L_{st}, \\ iii)\ \ \dfrac{k_BT}{L_{st}}\left[1-\dfrac{L_{st}}{L}+\dfrac{1}{4}\dfrac{L^2}{L_{st}^2}-\dfrac{1}{4}\right] & if\ x=L. \end{cases} \quad (9)$$

Similar to that for Eq. 1, Eq. 2 is modified to:

$$\frac{F(x)L_{st}}{k_bT}=\frac{1}{4}\left(1-\frac{x-L_{st}}{L}+\frac{F(x)}{K_0}\right)^2+\frac{x-L_{st}}{L}-\frac{1}{4}-\frac{F(x)}{K_0} \quad (10)$$

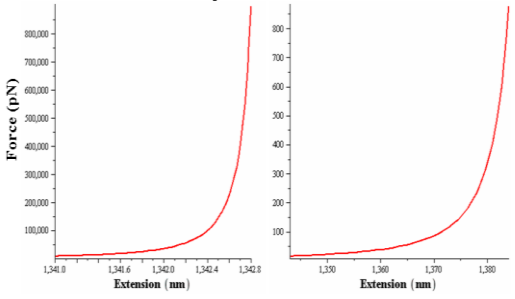
To confirm the accuracy of the reccorected stretching function in Eq.8, the dependence of the elastic force on the extension for plasmid DNA sample No.1 (see Tab.1) using original Eq. 1 and recorrected Eq.8 are presented in Fig. 3.



(a) *(b)*

Fig.3 Elastic force vs. extension (for sample No.1) using original function (a) and recorrected function (b).

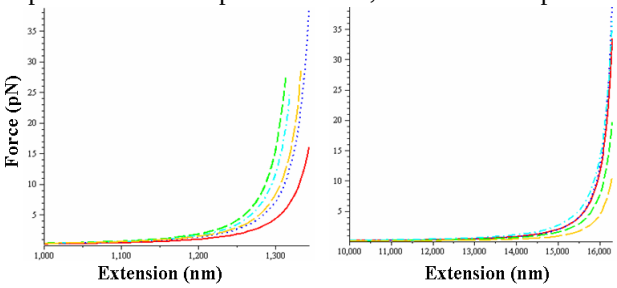
The elastic force near the contour length of 1343nm observed by Eq.1 reached a value of 10^5 pN in Fig. 3(a), larger than the stretch modulus of 10^3 pN, meanwhile, it is about of 16pN by the recorrected function Eq.7 in Fig.3 (b). To reach a value of elastic force as same as of the stretch modulus, the extension must exceed the contour length, at least stretched to 1385 nm in Fig.4 (b), which is the irreversible length [1]. Meanwhile, from Fig.4 (a) see that's when the extension is near the contour length, the elastic force is more larger then the stretch modulus. With above comments, it is clear that the recorrected function describes more accurate the elasticity of the DNA molecules.



(a) *(b)*

Fig.4 Elastic force vs. extension exceed contour length using original function (a) and recorrected function (b).

The dependence of elastic force on extension for the plasmid DNA with various ionic conditions are simulated by recorrected function and illustrated in Fig.5 (a), which show a certain value of elastic force at the contour length. Example, for plasmid DNA sample No.1, the maximum elastic force at contuor length is only 16pN, smaller than stretch modulus of about 10^3pN. Those stretch force of all samples of plasmid DNA change from 16pN to 40 pN, meanwhile their stretch modulus of about 10^3pN. This situation is similar also for λ-phage DNA with different ionic conditions in Fig.5 (b). Moreover, the simulated results in Fig.5b are in good agreement to that experimental ones in Fig.2. In detail, the stretch force at contour length of all samples of λ-phage DNA is smaller than 40pN. Although λ DNA's stretch modulus are not measured, but we can confirm that stretch force about of 40pN, which is comparable to that of plasmid DNA, should be acceptable.



(a) *(b)*

Fig.5 Elastic force vs. extension.

(a) Plasmid DNA sample:
No. 1 *(Red-solid);*
No. 2 *(Blue-dots) ;*
No. 3 (*Green-dash*);
No. 4 (*Cyan- dash dots*);
No. 5(*Orange-long dash*)

(b) λ DNA sample:
No. 6 (*Red-solid*);
No. 7 *(Blue-dots)* ;
No. 8 (*Green-dash*);
No. 9 (*Cyan- dash dots*);
No. 10 (*Orange-long dash*).

Summary, for all samples of DNA molecules, when its length is stretched to maximum (about of 1340 nm for samples from No.1 to 5 and of 16750 for samples from No. 6 to 10) the elastic force is reached a certain value ($\leq 40\,pN$). This force are different for other bio-molecules, example for α-helix deca-alamine protein stretch force reaches to 6000pN [1], but always determinated [6], [13]. With this force, there is an opportunity to simulate successfully the dynamic of DNA molecules in the optical tweezer, especially, when the interval between the anchor bead and the tweezer center is about or more then the contour length. Although slightly different from Eq.8, but Eq.10 should describe exactly the F-x characteristic of DNA molecules as well as that simulated by Eq.8.

IV. CONCLUSION

Some questions about the irregularity of the stretch function describing the dependence of the elastic force on extension of spring-like DNA molecules are discussed. Based on the experimental elastic parameters, previous stretch functions are analyzed to recorrect. The dependence of the elastic force on the extension is obtained for some

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samples of DNA molecules with various ionic conditions. The obtained results have confirmed the accuracy of stretch functions. They give us an usability for more exactly simulation of DNA dynamic in the optical tweezer.

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