ISSN: 2277-3754
ISO 9001:2008 Certified
International Journal of Engineering and Innovative Technology (IJEIT)
Volume 3, Issue 10, April 2014

Competition of Forces on Trapped Capability and Stability of DNA molecules in Optical Tweezer

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Abstract – The DNA molecules investigated by the optical tweezer is always linked to polystyrene bead, which is held at tweezer center by optical force. As often experiments, this bead is embedded in the fluid, which causes bead moves randomly (Brownian motion). The DNA molecules with bead have a certain elastic force when its extension is longer than the stable length, specially, this force is very large at contour length. To hold bead linking to DNA with stability at the contour length, it is necessary to choice suitable value of optical force, which is higher than the total force of elastic and Brownian ones. In this paper, we analyses the competition of all forces acting on DNA to find the structure conditions, mainly, suitable parameters of laser beam, for which the optical tweezer operates. The capability to trap bead linking to DNA and its stability at tweezer center are discussed based on the competition of all forces.

Index Terms **-Optical tweezer, molecular biophysics, spring-like DNA chain, Brownian motion, stability of bead.**

I. INTRODUCTION

Up to now, there are many works interested on using optical trap (or tweezer) to investigate force-extension characteristics of DNA molecules [1]-[11]. Based on the experimental values of elastic parameters, the stretch function describing the dependence of elastic force on the extension is approximately derived. To describe more exactly the nature of spring-like elastic DNA molecule, the stretch function has been recorrected [12]. In all experiments, the optical force used as the apply force is always attached to bead linking to DNA molecule and the extension of DNA molecule is controlled by the optical force. Unfortunately, this understanding can not be sufficient for trapping DNA molecules lying inside the trapping region. We can know that the elastic force is own one of DNA molecules. In trapping process this force is always opposite to the optical force and plays an important role. Moreover, the DNA molecules are often embedded in the specific fluid and then it is under action of the Brownian force. As well known, the optical force has space-time distribution depending on the total energy, beam waist's radius of laser beam [13], [14], so at different position of DNA molecules on the trapping region there is a competition between all forces, consequently, on it the trap's operation depends. This question has still not concerned in previous mentioned works, but it is necessary to interest in dynamics of DNA molecules under optical tweezer. In this paper, we present the discussions about the competition of optical, elastic and Brownian forces, and trapping capability of tweezer, firstly, based on the different qualities (peak intensity, beam waist) of used laser beam.

II. THE MODEL OF OPTICAL TWEEZER WITH FORCES ACTING ON DNA MOLECULES

A. *Often-experimental set-up of optical tweezer*

The simplest experimental geometry of an optical tweezer can be used as given in Fig. 1. We consider the laser beam TEM_{00} (*red*) focused to a spot with radius W_0 by optical objective with high aperture number, so that the peak intensity at spot center is I_0. A DNA molecule is anchored to glass cover slip through a polystyrene bead (*pink*) at one end, the opposite end linking to second bead (*cyan*), which will be held by laser beam. From here, the second bead is called driven bead. This DNA molecule and driven bead are embedded on the fluid.

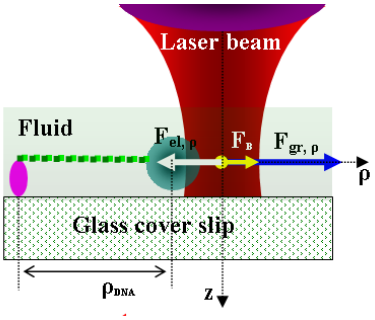

Fig.1: Simplest experimental geometry

Consider the spring-like DNA molecule has stable and contour lengths, L_{st} and L, respectively; the polystyrene microsphere (driven bead) has radius, a and refractive, n_b; and the fluid has refractive index, n_f and viscosity, η at temperature, T.

B. *Forces acting on the bead linking to DNA*

For simplicity, we consider thickness of fluid is about the diameter of the driven bead. Thus, we pay attention only to the motion of driven bead on the specimen plane (2D space), and the position of driven bead character by the radial distance from the tweezer center, $\rho = \sqrt{x^2 + y^2}$ (Note: in Fig.1 DNA is placed in the left of z-axis, so ρ has minus sign in this

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ISO 9001:2008 Certified
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approach). Moreover, the laser beam is seem as a plane wave in fluid, so the intensity distribution can be described by

$$I(\rho) = I_0 exp\left(-2\times\frac{\rho^2}{W_0^2}\right) \quad (1)$$

As shown in Fig.1, the following forces acting on the bead linking to DNA molecule:

The Brownian force, which is a source of random motion of bead, is given by [13]:

$$F_B = \sqrt{2k_B T\gamma}H(t) \quad (2)$$

where k_B is the Boltzmann constant, T is the absolute temperature, $\gamma = 6\pi a\eta$ is the friction coefficient, $H(t)$ is the unit vector of independent while Gaussian process, whose value changes in range $[-1,1]$ [14] . $H(t)$ describes the while noise with properties: the mean $\langle H(t)\rangle = 0$ for at all t; $\langle H^2(t)\rangle = 1$ for each value t; and $H(t_1)$ and $H(t_2)$ are independent of each other for $t_1 \neq t_2$ and $\overline{H(t_1)H(_2)} \square \delta(t_2 - t_1)$ [15]. Because of random process, the sign of Brownian force is random too, i.e. the direction of Brownian force can be same as or opposite to one of optical force.

The elastic force appears when the DNA molecule stretched to an extension longer than the stable length is given by [12]:

$$F(\rho_{DNA}) = -\frac{k_B T}{L_{st}}\left[\frac{\rho_{DNA} - L_{st}}{L} + \frac{1}{4}\frac{1}{\left[1-(\rho_{DNA}-L_{st})/L\right]^2} - \frac{1}{4}\right] \quad (3)$$

Note that if the anchor bead is placed with a distance L_0 (its sign is minus) from tweezer center, the extension of DNA molecule is relating to radial distance by $\rho_{DNA} = \rho - L_0$ (its sign is plus). The minus sign in Eq. 2, means that elastic force is opposite to optical force (see Fig.1).

The optical force acting on bead linking to DNA molecule is the transverse gradient force, which is given by [18], [19]:

$$\vec{F}_{gr,\rho}(\rho) = -\vec{\rho}2n_f\rho a^3 I_0\left(\frac{m^2-1}{m^2+2}\right)exp\left[-2\times\left(\frac{\rho}{W_0}\right)^2\right] \quad (4)$$

Where $m = n_b / n_f$ is the refractive index ratio? The sign of optical force is plus.

III. COMPETITION OF FORCES AND DISCUSSION ON TRAPPED CAPABILITY AND STABILITY OF DRIVEN BEAD

As shown in Fig.1, there are three forces acting on the driven bead, but the optical force plays trapping role, only. Before discussion the competition of all forces, trapped capability of tweezer, and stability of driven bead, we affirm that the tweezer will operate if optical force dominates over the sum of remain forces. That means that at any position, the driven bead can be manipulated to tweezer center if optical is high enough, so that

$$F_{tol} = F_{gr,\rho} + F_B + F_{el} > 0 .$$

We consider a simulated sample: i) λ-phage DNA molecule, whose elastic parameters of L_{st} =86 nm and L= 16700 nm with ionic condition of 1.86 mM Na^+ [9]; ii) The driven bead is polystyrene microsphere with radius of a=250 nm, refractive index of n_b= 1.57 [11], [16]; The fluid is water with refractive index of n_f=1.326, viscosity of $\eta=10^{-3}$ Ns/m [11], [17]; iv) The laser beam with wavelength of λ=1060 nm; v) The peak intensity and waist radius of laser beam, and the initial position of driven bead will be changed for particular discussed case. The first case, we consider the anchoring bead is placed at position as far aways as possible from the tweezer center, i.e. a distance equivalent to contour length of DNA molecular ($L_0 = L$), consequently, the driven bead is placed at initial position $\rho_{init} = L - L_{st} = -16614nm$. Using laser beam with peak intensity of $I_0 = 1\times10^2 W/cm^2$ and beam waist radius of $W_0 = 2\mu m$. The forces acting on driven bead at low stretched state of DNA are simulated and presented in Fig.2.

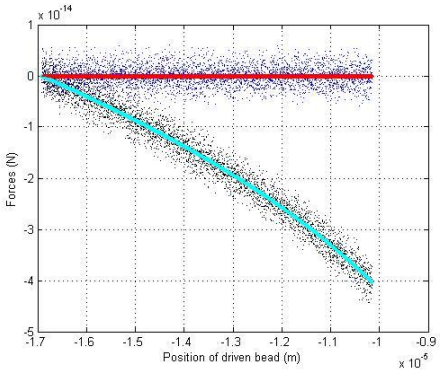

Fig.2: Forces vs. position of driven bead at low stretched state: optical (*red*), Brownian (*blue*), elastic (*cyan*), total (*black*) for case of $I_0 = 1\times10^2 W/cm^2$ and $W_0 = 2\mu m$.

From Fig.2, can see that, when driven bead is too far aways from the tweezer center, the optical force is very small, can be ignored, the Brownian oscillates in region $(-5\div5)\,fN$, the elastic dominates all remain forces, so the total force has minus value, i.e. the driven bead has tendency to move more far aways from tweezer center. When the driven bead is placed more and more near the tweezer center, i.e. at more stretched state, the optical tweezer does not operate till the bead's position reaches $\rho_{init} = -4.54\mu m$, where $F_{tol} > 0$ (Fig. 3). Thus, in this case, the optical tweezer will be operate (or bead will be trapped) if the initial position of driven bead is placed in the region $(-4.55\div0)\,\mu m$. This region will be called "trapping region".

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ISO 9001:2008 Certified
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Volume 3, Issue 10, April 2014

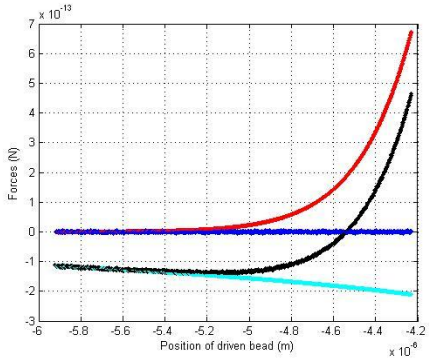
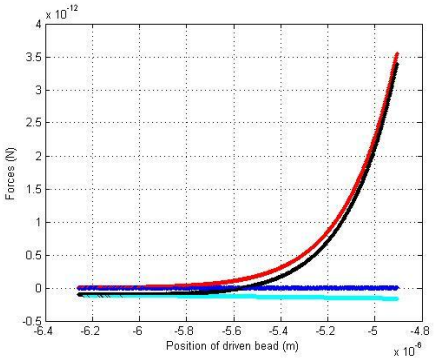
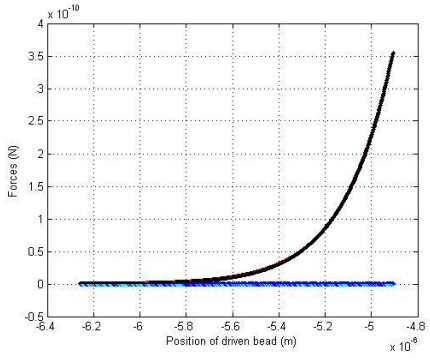


Fig.3: Forces vs. position in region (6.0÷4.2) µm for case of $I_0 = 1\times10^2 W/cm^2$ **and** $W_0 = 2\mu m$.

The trapping region increases with increasing of peak intensity: from $(-4.55\div0)\,\mu m$ in Fig.3 to $(-6.15\div0)\,\mu m$ in Fig.4b.



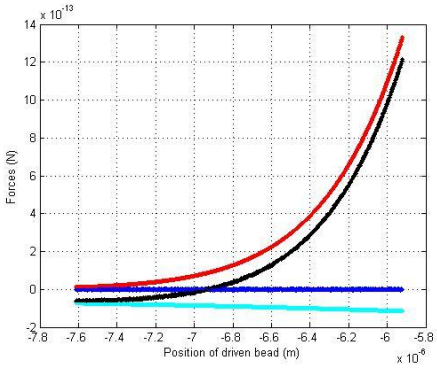
a



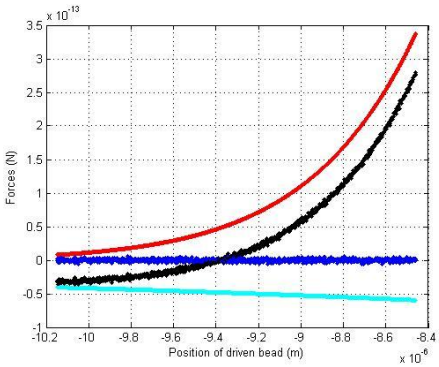
b

Fig.4: Operation region with different peak intensities a: $I_0 = 1\times10^4 W/cm^2$, b: $I_0 = 1\times10^6 W/cm^2 (W_0 = 2\mu m)$.

In the case of fixed peak intensity of $I_0 = 1\times10^2 W/cm^2$, but the beam waist radius increases, the trapping region increases too (see Fig.5): from $(-4.55\div0)\,\mu m$ in Fig.4 to $(-9.4\div0)\,\mu m$ in Fig.5b. Comparing results in Fig.4 and Fig.5, we can see that the expanding of trapping region with increasing of the beam waist is more speedily than with increasing of the peak intensity. To here, can say that, to enhance the trapped capability of the DNA molecules, it is priority to increase the beam waist. However, as well known, with fixed total energy of laser beam, the increasing of the beam waist leads to decreasing of the peak intensity, consequently, decreasing of stability of trapping bead in tweezer center [18], [19]. What will happen with driven bead linking to DNA molecules?



a



b

Fig.5: Operation region with different beam waist a: $W_0 = 3\mu m$, b: $W_0 = 4\mu m$ $(I_0 = 1\times10^2 W/cm^2)$.

In Fig.6 there is competition of forces in the region near the tweezer center for case of $I_0 = 1\times10^2 W/cm^2$, $W_0 = 2\mu m$, $L_0 = -17\mu m$.

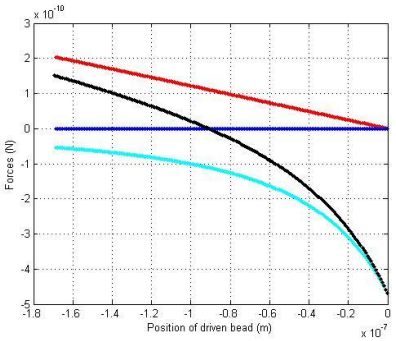


Fig.6: Forces vs. position near tweezer center for case of $I_0 = 1\times10^2 W/cm^2$, $W_0 = 2\mu m$, $L_0 = -17\mu m$

Can see that the driven bead is stable not at the center of tweezer, but at position from center a distance of $90nm$, where the $F_{tol} = 0$. This position will called "stable position" of driven bead, because of that the it oscillates around this position under Brownian force only [18], [19]. This situation appears because of that the elastic force speedily increases when the driven bead is more and more near tweezer center, meanwhile, the optical force decreases to zero. The stable position will shift more near tweezer center (at position of

ISSN: 2277-3754
ISO 9001:2008 Certified
International Journal of Engineering and Innovative Technology (IJEIT)
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$-3.5nm$) when the peak intensity increases to $I_0 = 1\times10^4 W/cm^2$ as shown in Fig.7.

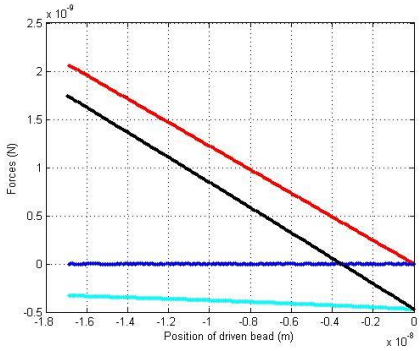

Fig.7: Forces vs. position near tweezer center for case of $I_0 = 1\times10^4 W/cm^2$, $W_0 = 2\mu m$, $L_0 = -17\mu m$

It necessary to note that, the stable position never overlaps the tweezer center. Only way making they overlap one other is to shift the anchoring bead near the tweezer center, so that the elastic force and optical force are smaller the Brownian force. As shown in Fig. 8, the stable position seems to overlap the tweezer center (with very short distance of $-8\,fm$), if the $L_0 = -2\mu m$.

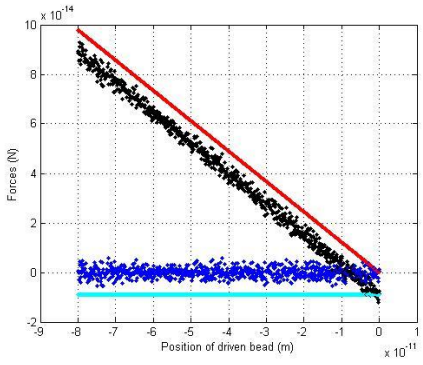

Fig.8 Forces vs. position near tweezer center for case of $I_0 = 1\times10^2 W/cm^2$, $W_0 = 2\mu m$, $L_0 = -2\mu m$

Here, it is necessary to pay attention that in all cases presented in Fig.6 ÷ Fig.8, the stable position is far from tweezer center a distance (the longest of $90nm$) much smaller than the radius of driven bead ($a=250nm$). As shown in works [18], [19], the bead is seem to be stable when it oscillates in the sphere of radius equivalent to its one. Thus, in our sample, the driven bead is always stable, even its initial position is far away from tweezer center a distance of $|L - L_{st}| = 16614nm$, i.e. when the DNA molecule is in the most stretched state.

IV. CONCLUSION

Under the operation conditions, the competition of all forces acting on the driven bead linking to DNA molecules, the trapping region, and stable position are discussed based on the simulated results for certain sample of optical tweezer. The obtained results show out and confirm the trapped capability and stability of driven bead linking to DNA molecule with collection of suitable parameters. The parameters as peak intensity, beam waist of laser beam, the stable length, contour length, and initial position of DNA molecule, and radius of driven bead,… used here will be sufficient for simulation process the dynamics of DNA molecules in the optical tweezer, moreover, they are useful for experiments. However, in this paper we have paired only attention on same of principle parameters in the simplest model of optical tweezer. The question will be complex when the bead hangs in fluid. This question will be concerned in simulation process the dynamics of DNA molecules.

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