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Spontaneous formation of non-uniform double helices for elastic rods under torsion

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ABSTRACT

The spontaneous formation of double helices for filaments under torsion is common and significant. For example, the research on the supercoiling of DNA is helpful for understanding the replication and transcription of DNA. Similar double helices can appear in carbon nanotube yarns, cables, telephone wires and so forth. We noticed that non-uniform double helices can be produced due to the surface friction induced by the self-contact. Therefore an ideal model was presented to investigate the formation of double helices for elastic rods under torque. A general equilibrium condition which is valid for both the smooth surface and the rough surface situations is derived by using the variational method. By adding further constraints, the smooth and rough surface situations are investigated in detail respectively. Additionally, the model showed that the specific process of how to twist and slack the rod can determine the surface friction and hence influence the configuration of the double helix formed by rods with rough surfaces. Based on this principle, a method of manufacturing double helices with designed configurations was proposed and demonstrated. Finally, experiments were performed to verify the model and the results agreed well with the theory.

1. Introduction

It is commonly observed that a twisted yarn tends to writhe and form a double-helical structures. The formation of double helices for twisted filaments is of great significance and it has attracted attention from various fields. The formation of supercoiling for DNA chains under torsion has been investigated broadly [1–5]. Neukirch and Purohit have investigated plectonemes with uniform pitch in DNA taking electrostatic interactions into account [6,7]. Van der Heijden and Purohit have considered plectonemes with non-uniform helical pitch [8,9]. Y. Shang obtained the double helices of carbon nano-tube (CNT) yarns by simply twisting and slacking it, which have unique electrical and mechanical properties [10–12]. The superconductor made from the double helix of CNT yarns have been investigated broadly [13]. Besides, the double helix of carbon or polymer fibers can be fabricated into the artificial muscle, which, as a new concept, have recently attracted wide attention [14,15]. In engineering, cables under torsion may form loops and double helices, in which the large deformation may damage the cables [16,17].

Two main methods have been proposed to investigate the spatial writhing of twisted filaments. The first is to simplify the filament or polymer chain as an ideal elastic rod. Based on this elastic-rod assumption, the initial buckling and localized post-buckling, prior to self-contact, of a twisted elastic rod have been widely investigated by using the Kirchhoff model [18–22]. The self-contact for the two strands of double helices was studied by some scholars as well [23–26]. The other method mainly focuses on microscopic polymer chains. To describe the statistical property of polymer chains, the Kratky–Porod model, free jointed chain model and worm like chain model were put forward [27]. The statistical properties of the supercoiling of DNA chains can be described well with these models [2,28].

Although the self-contact is considered in some elastic-rod models, most scholars still neglected the surface friction [23,22]. Without considering the surface friction, the double helix solved by whether the Kirchhoff model or the variational method will have a uniform double helix (if the slight deviation near the ends

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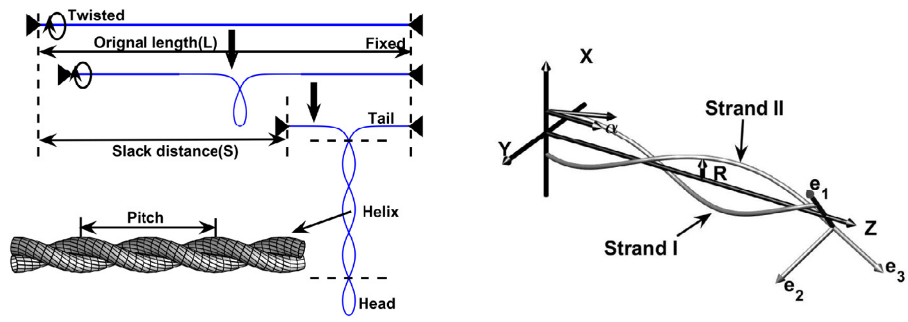

(a) (b)

Fig. 1. (a) Schematic of the formation process of the double helix. One end is fixed while the other end can be slacked and twisted. The whole elastic rod is divided into three parts: head, helix and tail. The pitch the double helix are illustrated. (b) Central lines of the double helix. α is the angle between the tangent vector of the helix and the z axis. R is the radius of the double helix central lines. $\mathbf{e}_3$, $\mathbf{e}_1$ and $\mathbf{e}_2$ are the unitary vector in the directions of $\mathbf{r}'$, $\mathbf{r}''$ and $\mathbf{r}' \times \mathbf{r}''$ respectively.

is neglected). However, we noticed in most cases the surface friction is not negligible. On the contrary, it may have a great influence on the configuration and mechanical properties of the double helices. A typical non-uniform double helix can be obtained by twisting a rubber rod first and then bringing its two ends together. In the work of Y. Shang et al. [10–12], the double helices of CNT yarns obtained by similar twist-slacking process shown non-uniformity as well.

To research the formation of double helices for rods under torque. First, it can provide a general understanding of the supercoiling formation of DNA chains. Furthermore, it has potential in controlling the fabrication of the double helices of CNT yarns which can serve as high-performance electronic and mechanical devices, for example, the superconductors and artificial muscles. Besides, in engineering, it can be used to analyze and avoid the double helix formation for cables.

In this article, based on the ideal elastic rod model, the variational method is used to derive the general equilibrium condition for the double helix. This condition is valid for both the smooth surface and the rough surface situations. By adding a inter-strand interaction term in the total potential energy, both the self-contact and non-self-contact situations are considered. Different from previous non-friction assumptions, the influence of the surface friction is investigated here. It is found that the surface friction will greatly influence the configuration of the double helix, in which case, non-uniform double helices can be formed. Moreover, the specific process of how the rod is twisted and slacked can determine the surface friction and therefore influence the configuration of the double helix. Based on this property, a method of producing double helices with designed configurations is proposed. Experiments are preformed to verify the validity of this model and demonstrate the method of producing a double helix with a designed configuration.

2. Model

2.1. General theory

In this section, the general properties of the double helices are investigated. By using the variational approach based on the energy minimization principle, the general equilibrium condition can be obtained. Fig. 1(a) shows the schematic of the formation process of the double helix. Here, we call this procedure the twist-slacking method so as to distinguish it from the conventional twist-spinning method [13,5]. To simplify the problem and obtain an ideal model, 5 fundamental assumptions are made as follows:

(1) The rod is inextensible with a fixed length L. It has a circular cross section with a fixed radius r.
(2) The elasticity of the rod is linear. The twisting and bending are uncoupled. The linear-elasticity assumption can be satisfied well in our experiments. See more details in the experiment section.
(3) The rod can be roughly divided into three parts, as shown in Fig. 1(a), namely the tail, helix and head. Since we mainly focus on the behavior of the helix part, the influence of the head is neglected here and the tail is assumed to be straight and uniform. This assumption can be perfectly satisfied when the helix is long enough. The radius of the double helix composed by the central line of the rod is R, as shown in Fig. 1(b).
(4) The rod is quasi-static during the whole slack process.
(5) No dissipative force exists in the formation process, including the sliding friction. However static friction is allowed.

Then we describe the geometry of the double helix quantitatively. According to assumption 3, all the slack distance S can be transformed into the length of the two strands in the double helix, as illustrated in Fig. 1(a). Assume the double helix extends in the positive z-axis direction so that the two strands are symmetric about the z-axis, as shown in Fig. 1(b). Then the position vector describing the whole central line of the double helix can be written as

$$\mathbf{r}(\theta) = \begin{cases} \left(-R\cos\theta, R\sin\theta, \int_0^\theta \frac{P}{2\pi} d\theta \right) & (\theta \geq 0, \text{ Strand I}) \\ \left(R\cos\theta, R\sin\theta, \int_\theta^0 \frac{P}{2\pi} d\theta \right) & (\theta < 0, \text{ Strand II}) \end{cases}, \quad (1)$$

where θ defines the angle that the helix rotates by and P is the pitch of the helix (shown in Fig. 1(a). See the exact definition in Ref. [29]). Note the two strands are jointed at the head, and thus $\theta \geq 0$ and $\theta < 0$ correspond to the Strand I and Strand II respectively. Here, we will also use the natural coordinate s with its origin located at $\mathbf{r}(0)$. It represents the distance along the center line. Then $-S/2 \leq s < S/2$ corresponds to the double helix, and $S/2 \leq |s| < L/2$ corresponds to the tails. For the helix part we have

$$ds = \sqrt{R^2 + \left(\frac{P}{2\pi}\right)^2} d\theta. \quad (2)$$

The curvature κ and the torsion τ can be calculated as follows

$$\kappa = \frac{|\dot{\mathbf{r}} \times \ddot{\mathbf{r}}|}{|\dot{\mathbf{r}}|^3}, \tau = \frac{(\dot{\mathbf{r}} \times \ddot{\mathbf{r}}) \cdot \dddot{\mathbf{r}}}{|\dot{\mathbf{r}} \times \ddot{\mathbf{r}}|^2}, \quad (3)$$

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