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Coupling between axial stretch and bending/twisting deformation of actin filaments caused by a mismatched centroid from the center axis

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ABSTRACT

A cytoskeletal actin filament with a spirally arranged centroid (a biopolymer with a double helical structure) exhibits mechanically interesting phenomena, such as tensile-twisting coupling behavior involved in the binding of actin-related proteins. To describe this mechanical behavior of the actin filament, we propose a Cosserat continuum model by focusing on the mismatch between the centroid and the center axis. We derive the equations of motion based on the variational principle and discuss the coupling behavior caused by the mismatch, which is responsible for interesting couplings between axial stretch and bending/twisting deformation. The proposed model can express the mechanical behavior of actin filaments with a spirally arranged centroid mismatched from its center axis, through which we can explore the fundamental filament-level mechanism of an actin cytoskeleton in relation to the mechanical regulation of biological functions.

1. Introduction

A helical structure is often observed in biopolymers such as DNA double strands, cytoskeletal actin filaments, and collagen fibers [1–3]. These structures are related to a variety of biological functions. For example, the double helical structure of DNA is closely related to essential biological activities, such as chromatin organization [4], transcription regulation [5], and relaxation inhibition of torsional stress [6]. Twisted biopolymers, including actin, fibrin, and collagen, are also thought to influence many biological functions [7,8].

The actin filament targeted in this article is abundant in many types of eukaryotic cells [9], and is often the principal determinant of cell elasticity and mechanical stability, thus playing important roles in cell shape maintenance [10–12], cell motility [13–15], and cell adhesion [16–18]. The helical structure of actin filaments, as with other filamentous biopolymers, yields an interesting mechanical coupling behavior. For example, tensile force causes mechanical distortion of the single actin filament [19]. In addition, the actin filament structure has a mismatch between the centroid and the center axis, which may exhibit more complex and interesting phenomena related to biological functions.

We consider the actin filament as an elastic rod with a mismatched centroid. This mismatched structure is attributed to the cross-sectional geometry of the rod, similar to the asymmetry of the rod cross-sections. The mismatched structure influences the mechanical characteristics of the rod; for instance, the first area moment does not vanish when subjected to bending, but exhibits additional interactions between axial stretch and bending/twisting deformation. Therefore, it is important to study these interesting interactions caused by a mismatched structure from the mechanical standpoint.

This article focuses on the mismatch between the centroid and the center axis, and proposes a Cosserat theoretical continuum model of a single actin filament whose center axis does not coincide with the centroid. Then, we investigate how the mismatch appears in the equations of motion, derived from the variational principle, and discuss its significance in cell and molecular biomechanics.

2. Cosserat theoretical description of actin filament

2.1. Centroid mismatched from center axis of actin filament

The actin filament consists of an enormous number of atoms and exhibits a complex structure, as shown in Fig. 1(a) by a ribbon

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Nomenclature

$\mathcal{F}^0$, $\mathcal{C}^0$	filament and axial curve in the reference configuration
S	arclength parameter of $\mathcal{C}^0$
$\boldsymbol{R}$, $\tilde{\boldsymbol{R}}$	position vectors of a point on $\mathcal{C}^0$ and in $\mathcal{F}^0$
$\{\boldsymbol{D}_1, \boldsymbol{D}_2, \boldsymbol{D}_3\}$	right-handed orthonormal basis along $\mathcal{C}^0$
$\mathbf{K}$	curvature vector associated with $\mathcal{C}^0$
K, T	geometric curvature and torsion of $\mathcal{C}^0$
$\mathcal{F}$, $\mathcal{C}$	filament and axial curve in the current configuration
s, t	arclength parameter of $\mathcal{C}$ and time parameter
ρ	mass density of the filament
$\boldsymbol{r}$, $\tilde{\boldsymbol{r}}$	position vectors of a point on $\mathcal{C}$ and in $\mathcal{F}$
$\{\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{d}_3\}$	right-handed orthonormal basis along $\mathcal{C}$
$\boldsymbol{Q}$	rotation matrix transforming $\boldsymbol{D}_k$ to $\boldsymbol{d}_k$
$\boldsymbol{v}$	velocity of the filament
$\boldsymbol{\omega}$	angular velocity of the filament
ε	extension of $\mathcal{C}$
$\boldsymbol{e}$	strain of the filament
$\boldsymbol{\kappa}$	curvature vector associated with $\mathcal{C}$
κ, τ	geometric curvature and torsion of $\mathcal{C}$
Φ	action integral
$\mathcal{W}$	strain energy density
$\mathcal{T}$	kinetic energy density
$\boldsymbol{C}$	rigidity tensor
$\boldsymbol{I}_1$, $\boldsymbol{I}_2$	analogs of the first and second area moments
$\boldsymbol{I}_2^{\boldsymbol{C}}$	$\boldsymbol{C}$- associated inertia tensor
Ω_s	cross-section of the current filament at s
$dA = dX_2 dX_3$	area element of the current cross-section Ω_s

representation. Fig. 1(b) shows the coarse-grained actin filament from a macroscopic perspective, clearly illustrating its helical structure. In addition, the actin filament appears to have a mismatch between its centroid and its center axis. Thus, we can model it as an elastic rod with the centroid mismatched from the center axis, as shown in Fig. 1(c).

Fig. 2 confirms that the centroid of the actin filament does not coincide with the center axis. Indeed, the curved line connecting the center-of-masses of each cross-section of the actin filament is not situated in its geometric center. The center-of-mass of each cross-section deviates ~ 2 nm in average from the geometric center of the filament, which is $\sim 50\%$ of the radius (3–5 nm) of the approximating rod. The continuum model, in which the actin filament is viewed as an elastic circular rod, is useful, but seems simplified. Considering its kinematics, we extended it to a model of an elastic rod with a spirally arranged centroid mismatched from the center axis.

2.2. Kinematics of Cosserat theoretical model of actin filament

In this section, we set up a geometrical description of the single actin filament on the basis of the Cosserat continuum theory [20,21]. Let $\mathcal{F}^0$ and $\mathcal{C}^0$ be the filament lying in the three dimensional Euclidean space $\mathbb{R}^3$ with the standard basis $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ and its axial curve in the reference configuration, respectively. We regard $\mathcal{C}^0$ as a smooth, non-intersecting curve with the arc-length parameter S that varies over an interval $[0, L] \subset \mathbb{R}$. Thus, when we denote a position of a point on $\mathcal{C}^0$ by $\boldsymbol{R}(S)$, it holds that $\|d\boldsymbol{R}/dS\| = 1$ for the arbitrary $S \in [0, L]$. Here, $\|\cdot\|$ denotes the Euclidean norm. In the case of double helical polymers such as the actin filament and DNA, we may consider the axial curve as the average of the two backbones.

We take a right-handed orthonormal basis, $\{\boldsymbol{D}_1(S), \boldsymbol{D}_2(S), \boldsymbol{D}_3(S)\}$, as shown in Fig. 3, along $\mathcal{C}^0$ at S such that the vector

$$\boldsymbol{D}_1 = \frac{d\boldsymbol{R}}{dS}, \tag{1}$$

is the unit tangent to the axial curve $\mathcal{C}^0$ and $\boldsymbol{D}_2$ and $\boldsymbol{D}_3$ are the unit normal and binormal vectors to $\mathcal{C}^0$, respectively. Then, the position vector $\tilde{\boldsymbol{R}}$ of each point in $\mathcal{F}^0$ is given by

$$\tilde{\boldsymbol{R}}(X_\alpha, S) = \boldsymbol{R}(S) + X_\alpha \boldsymbol{D}_\alpha(S), \tag{2}$$

in which X_α ($\alpha = 2, 3$) are coordinates on each cross-section along $\boldsymbol{D}_\alpha(S)$. We assume that $\|X_\alpha\| \ll L$, $\alpha = 2, 3$; thus, we consider the filament $\mathcal{F}^0$ as a three-dimensional "slender" body. Throughout this article, the summation convention is used for repeated indices, with Latin indices taking the values $\{1, 2, 3\}$ and Greek indices taking the values $\{2, 3\}$.

We define the curvature vector $K(S)$ through

$$\frac{d\boldsymbol{D}_k}{dS} = \mathbf{K} \times \boldsymbol{D}_k, \tag{3}$$

so that the first and third components $\mathcal{K}_1 = \langle \boldsymbol{D}_1, \mathbf{K} \rangle = T$ and $\mathcal{K}_3 = \langle \boldsymbol{D}_3, \mathbf{K} \rangle = K$ of the curvature vector $\mathbf{K}$ give the geometric torsion and curvature of $\mathcal{C}^0$, respectively, and the second component $\mathcal{K}_2 = \langle \boldsymbol{D}_2, \mathbf{K} \rangle$ is identically zero. Here, we denoted the standard inner product on the Euclidean space $\mathbb{R}^3$ by $\langle \cdot, \cdot \rangle$.

We denote the actin filament and its axial curve in the current configuration, respectively, by $\mathcal{F}$ and $\mathcal{C}$. We parameterize a

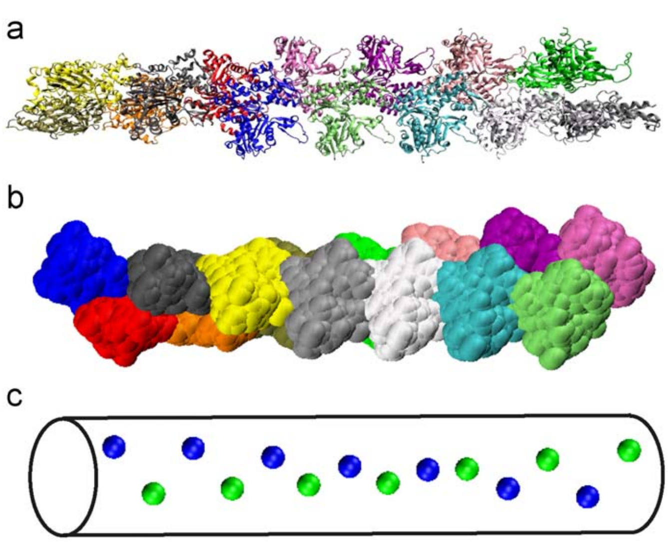

Fig. 1. Illustration of a half pitch of an actin filament consisting of 14 monomers: (a) ribbon representation, (b) coarse-grained description, and (c) its continuum rod model with plots of the center-of-mass of 14 actin monomers.

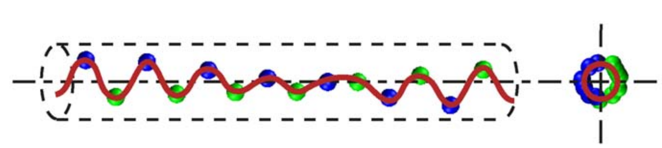

Fig. 2. Illustration of the centroid of the actin filament (left) and their projection to a transverse section (right). A curved line in the left figure and a circle in the right one denote the centroid. They pass through the center-of-masses of actin monomers, and mismatch from the center axis of the filament, namely the dashed–dotted line in the left figure and center point in the right one.