Collective dynamics of Active Filament Complexes

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Networks of biofilaments are essential for the formation of cellular structures and they support various biological functions. Previous studies have largely investigated the collective dynamics of rod-like biofilaments; however, the shapes of actual subcellular components are often more elaborate. In this study, we investigated an active object composed of two active filaments, which represents a progression from rod-like biofilaments to complex-shaped biofilaments. Specifically, we numerically assessed the collective behaviors of these active objects and observed several types of dynamics depending on the density and the angle of the two filaments as shape parameters of the object. Among the observed collective dynamics, moving density bands that we named ‘moving smectic’ are reported here for the first time. By using statistical analyses of the orbits of individual objects and the interactions among them, the mechanisms underlying the rise of these dynamic patterns in the system were determined. This study demonstrated how interactions among active biofilaments with complex shapes could produce collective dynamics in a non-trivial manner.

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I. INTRODUCTION

Organized networks of biofilaments such as microtubules and actin fibers play essential roles in the formation, maintenance, and alteration of cell structures [1]. For example, cortical microtubules in plant cells exhibit aligned structures called ‘bundles’, which mechanically support the cells [2–5]. These subcellular structures composed of biofilaments are usually formed through active processes accompanied by the use of energy in hydrolysis. Polymerization and depolymerization result in the microtubules changing their length and colliding with each other, which leads to their global alignment. Another active mechanism involves interactions between biofilaments and molecular motors; when the molecular motors bind to the filaments and march along them, active forces act on the filaments and drive the formation of spatio-temporal filament patterns [6–10]. To date, several in vitro experiments have revealed various types of structure resulting from this motor activity [11–13]. For example, filaments form locally ordered patterns, such as ray-like asters and vortices, depending on the type and concentration of molecular motors [14–17]. In addition, the collective motion of biofilaments can emerge via their active interaction with each other, which is an interesting paradigm of ‘active matter’ [18–20].

Many theoretical studies have attempted to address the self-organization of active filaments. Based on the contracting force of active filaments driven by molecular motors, coarse-grained and continuum kinetic equations were proposed to explain the inhomogeneous accumulation of filaments (i.e., bundles) [24, 25] and local structures such as vortices and asters [26]. Similar global patterns appeared in another continuum model in which nematic collisions were taken into account [27–31]. To explain the emergence of vortices and asters from microscopic processes, Aranson and Tsimring introduced simple stochastic rules for inelastic collisions of biofilaments and, thus, derived continuum equations by which transport coefficients could be related to microscopic physical quantities [32, 33]. Aranson’s group performed Monte Carlo simulations of the elementary alignment processes to verify their theory [34]; however, a correspondence with continuum theory remains elusive. In other studies simulating the dynamics of filaments, new patterns, including stripes, were found [35], and the viscoelasticity of networks of biofilaments was discussed [36].

The majority of previous studies mainly considered objects with rod-like shapes as the simplest biofilaments. However, in vivo, filaments often bind to each other with additional related molecules and form molecular complexes, which constitute a functional unit in various biological processes. For instance, microtubules on mitotic spindles elongate radially from a pair of centrosomes, which separate a mother cell into two daughter cells [37]. Beneath the apical membrane of a multi-ciliated cell, the root of the cilium, i.e., the basal body, has an appendage known as the basal foot that functions as a microtubule organizing center. Microtubules are generated from basal feet and subsequently connect with each other and be-

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come organized as a cell-sized network, which is suggested to be involved with the ordered alignment and direction of beating cilia \[32\,33\]. In this example, microtubules that are pivoted by the basal body can act as a functional unit, and their interaction may lead to alignment of the cilia. However, the mechanisms underlying the function of such biofilament complexes, especially the relationship between the shape of the molecular complexes and their emerging dynamics, remain largely unknown.

To gain fundamental insights into these mechanisms, in the present paper we perform numerical simulations of molecular complexes composed of two filaments, named ‘active filament complexes (AFCs)’, which represents a simple investigative progression from rod-like filaments to complex-shaped filaments. In our model, the active interactions of filaments via molecular motors are considered, whereas collisions and excluded volume interactions are ignored. We find that, depending on the density and shape of AFCs, interesting dynamics arise, among which ‘moving smectic’ (described in detail later) represents a new form of dynamics not previously reported. By tracking orbits and investigating AFC interactions, we also study the mechanisms of how various dynamic patterns arise in the system.

The remaining sections of this paper are organized as follows. The detailed model is described in Sec. II In Sec. III the observed dynamics in numerical simulations are classified according to quantities such as ferromagnetic (polar) and nematic (apolar) order parameters. By tracking individual AFCs and characterizing the crossing of filaments, analyses are performed from Sec. IV to Sec. VII. The dynamics of the modified model system are briefly discussed in Sec. VIII. Finally, a comparison with earlier studies and the potential for future experiments are discussed in Sec. IX.

II. MODEL

A. Dynamics of single active filaments

To model the dynamics of single active filaments, the formulation given by Tanase \[40\] was followed. In this formulation, a biofilament is described as a single rod diffusing in viscous liquid. Each filament possesses polarity associated with its elongating direction from the minus to plus end. Therefore, \(3N\) variables are sufficient for representing the configuration of the microtubules, i.e., their center position, \(\mathbf{R}_i = (x_i, y_i)\), and their plus end’s direction, \(\theta_i \in [0, 2\pi]\) [Fig. I(a)]. According to polymer physics, the Brownian motion of these filaments is governed by

\[
\dot{\mathbf{R}}_i = g_{\parallel}(t)\mathbf{U}_i + g_{\perp}(t)\mathbf{V}_i \\
\dot{\theta}_i = g_{\text{rot}}(t),
\]

where \(\mathbf{U}_i = (\cos \theta_i, \sin \theta_i)\) and \(\mathbf{V}_i = (-\sin \theta_i, \cos \theta_i)\) are unit orientational vectors each parallel and perpendicular to the filament \(i\), and \(g_{\parallel}(t), g_{\perp}(t),\) and \(g_{\text{rot}}(t)\) represent Gaussian white noise with the following statistics: \(\langle g_{\parallel}(t) \rangle = \langle g_{\perp}(t) \rangle = \langle g_{\text{rot}}(t) \rangle = 0\), \(\langle g_{\parallel}(t)g_{\parallel}(t') \rangle = 2D_{\parallel}\delta(t-t')\), \(\langle g_{\perp}(t)g_{\perp}(t') \rangle = 2D_{\perp}\delta(t-t')\), and \(\langle g_{\text{rot}}(t)g_{\text{rot}}(t') \rangle = 2D_{\text{rot}}\delta(t-t')\). The diffusion coefficients \(D_{\parallel}, D_{\perp}\), and \(D_{\text{rot}}\) are dependent on the temperature \(T\) and the length of filaments \(\ell\): \(D_{\parallel} = 2D_{\perp} = \frac{k_B T ln \ell}{2\pi \eta D}\) and \(D_{\text{rot}} = \frac{\pi \eta}{\ell} \frac{1}{2}\). In the model, filament length \(\ell\) is fixed by ignoring polymerization and depolymerization. For simplicity, we approximate \(D = D_{\parallel} \approx D_{\perp}\) since their difference is only a factor of 2.

Interaction between two single filaments is formulated as follows. In the cell cytoplasm or solvents, many molecular motors such as kinesin and dynein bind to the filaments. While kinesin binds, a sliding motion occurs along the filament from the minus to the plus end. Because most molecular motors bind to the filaments by multiple binding heads, when two crossing filaments are simultaneously bound, the sliding of the motors results in mechanical torque that orients the two filaments by generating the tension \(T_m\) in a process known as ‘zippering’ [Fig. I(b)] \[2\,42\]. Here, we assume that the direction

\begin{figure}[h]
\centering
\includegraphics[width=\linewidth]{fig1.png}
\caption{Schematic representations of the interaction between filaments and active filament complexes (AFCs). (a) Configuration of crossing single filaments. (b) Possible alignment of crossed filaments (‘zippering’). (c) AFC with shape angle \(\theta\) and length \(\ell\). Each filament is named as an L- or R-filament. (d) Interactions of AFCs. Red points represent the center of filaments. Blue points are the centers of mass of an AFC. (e) Possible alignment of crossed AFCs.}
\end{figure}
of the zippering force generated by molecular motors only depends on the relative angles of the filaments and that the torque acting on these filaments should be consistent with the force [Fig. 1(a) and (b)] [40]. The interaction of the torque acting on these filaments should be consistent as long as the density of the molecular motors [33]. For simplicity, we ignore the excluded volume effects and the shape of the filaments, which is sufficiently long.

The tension of molecular motors acting on the crossing filament depends on the concentration is sufficiently high, so that motors bind to the crossing filament at a constant rate and slide along them; consequently, $T_m$ is a constant parameter depending on the density of the molecular motors [33]. For simplicity, we ignore the excluded volume effects and the shape of the filaments, which is sufficiently long.

\[ \dot{R}_{ij} = \frac{T_m}{\pi \zeta} (U_{ij} - U_{ij}) \]  

\[ \dot{\theta}_{ij} = \frac{T_m}{\pi \zeta_{rot}} \left[ (R_{i} - R_{ij})_{x}(U_{ij})_{y} + (R_{j} - R_{ij})_{y}(U_{ij})_{x} \right] \]

where $R_c$ is the crossing point of the two filaments $i$ and $j$. Friction coefficients $\zeta$ and $\zeta_{rot}$ are derived from the Einstein relations as $D = \frac{k_B T}{\zeta}$ and $D_{rot} = \frac{k_B T}{\zeta_{rot}}$, respectively. The tension $T_m$ depends on the concentration of molecular motors in the environment. We assume that the concentration is sufficiently high, so that motors bind to the crossing filament at a constant rate and slide along them; consequently, $T_m$ is a constant parameter depending on the density of the molecular motors [33]. For simplicity, we ignore the excluded volume effects and the collision process, although both of these may contribute to apolar alignment [29, 31].

B. Model for AFCs

To study the dynamics of active filaments with shape, the model equations for active filaments were extended as follows. As a simple AFC, we consider an object to which two filaments are anchored on their minus end [Fig. 1(c)]. Hereafter, left and right filaments are called L- and R-filaments, respectively.

We assume that the mass of the anchoring object is negligibly small compared to that of the filaments, and the motion of two filaments dominates the dynamics of AFCs. Consider that an AFC is composed of $i$-th and $k$-th filaments, and the $i$-th filament crosses the $j$-th filament in another AFC [Fig. 1(d)]. Since the center of inertia of the AFC becomes $(R_{i} + R_{j})/2$, the equation for $\dot{\theta}_{i,k}$ is modified into

\[ \dot{\theta}_{i,k} = \frac{T_m}{\pi \zeta_{rot}} \left[ (R_{cross} - R_{i} + R_{k})_{x} (U_{i} - U_{ij})_{y} - (R_{cross} - R_{i} + R_{k})_{y} (U_{i} - U_{ij})_{x} \right] \]

\[ = \frac{T_m}{\pi \zeta_{rot}} \left[ (R_{i} - R_{j})_{x} (U_{j})_{y} - (R_{j} - R_{i})_{y} (U_{j})_{x} + (R_{i} - R_{k})_{x} (U_{j} - U_{i})_{y} - (R_{i} - R_{k})_{y} (U_{j} - U_{i})_{x} / 2 \right] \]

The equation for $\dot{R}_i$ is changed so that $\dot{R}_i = \dot{R}_{ij}$ [Fig. 1(d)]. This model is referred to as the light-anchor model. Another interesting limit of the AFC model occurs where the anchor is much heavier than the attached filaments. We refer to this case as the heavy-anchor model and provide some related results in Sec. VII.

Numerical simulations of AFCs are performed in two-dimensional systems with periodic boundary conditions. Initial states of AFCs are set to obey spatially and orientationally uniform distributions. The system size is fixed as $L \times L = 20 \times 20$. To evaluate the effect of the AFCs shape on collective dynamics, parameter $\theta_a$ is controlled. The density of AFCs is also controlled by changing the number of AFCs, $N$. The other parameters are fixed as follows: the filament length $\ell = 2.0$, the translational and rotational diffusion constants $D = 0.001$ and $D_{rot} = 0.006$, the effective temperature $k_B T = 1.0$, and the tension of molecular motors acting on the crossing filament $T_m = 0.3$. Simulation time is taken as $t = 1000$, which is sufficiently long.

![FIG. 2. Snapshots of simulation results.](image-url)

(a) Positional direction $\theta_a$ is defined by the direction bisecting two filaments for each AFC. (b) Color code for the positional direction. (c)–(f) Snapshots of simulation results at indicated parameter values. Filaments are colored by their positional direction.
III. COLLECTIVE MOTIONS OF AFCS

Several types of collective behaviors were observed depending on the angle \( \theta_a \) and density \( \rho = N/L^2 \). In Fig. 2, examples of observed dynamics are shown in snapshots at indicated parameters values. Each filament is colored by the direction as indicated in Fig. 2(a) and (b). As we will see below, the dynamics are classified into four phases: globally ferromagnetic [Fig. 2(c)], moving smectic [Fig. 2(d)], disorder [Fig. 2(e)], and locally nematic [Fig. 2(f)] patterns.

For characterizing and classifying the observed dynamics, the orientation order parameters are the most significant quantities. Positional direction \( \theta_a \) is defined for each AFC \( (\alpha = 1, 2, \cdots, N) \) as the direction of bisecting the two filaments [Fig. 2(a)]. Ferromagnetic (polar) and nematic (apolar) parameters, \( R_1 \) and \( R_2 \) are defined by

\[
R_1 = \frac{1}{N} \sqrt{\sum_{\alpha=1}^{N} \cos \theta_{\alpha}^2 + \sum_{\alpha=1}^{N} \sin \theta_{\alpha}^2},
\]

\[
R_2 = \frac{1}{N} \sqrt{\sum_{\alpha=1}^{N} \cos 2\theta_{\alpha}^2 + \sum_{\alpha=1}^{N} \sin 2\theta_{\alpha}^2}.
\]

In some parameter regions, the system does not exhibit global order but shows strong directional alignment in neighbors [Fig. 2(f)]. To detect such locally ordered patterns, we divide the system into a 10 \( \times \) 10 regular lattice, measure ferromagnetic and nematic order parameters in each region, and then average their values. These local order parameters \( lR_1 \) and \( lR_2 \) are thus given as

\[
lR_1 = \frac{1}{100} \sum_{j=1}^{100} \frac{1}{N_j} \sqrt{\sum_{\alpha=1}^{N_j} \cos \theta_{\alpha}^2 + \sum_{\alpha=1}^{N_j} \sin \theta_{\alpha}^2},
\]

\[
lR_2 = \frac{1}{100} \sum_{j=1}^{100} \frac{1}{N_j} \sqrt{\sum_{\alpha=1}^{N_j} \cos 2\theta_{\alpha}^2 + \sum_{\alpha=1}^{N_j} \sin 2\theta_{\alpha}^2}.
\]

Here, \( N_j \) indicates the number of AFCs in the \( j \)-th lattice \( (j = 1, 2, \cdots, 100) \). These quantities are shown on a color-scale in Fig. 3.

The system shows spatial and temporal regularity in the moving smectic phase [Fig. 2(c)]. To characterize spatial dynamics, another index, \( S \), is defined as the average of \( \sin^2 \theta_p \), where \( \theta_p \) is the angle between contacting AFCs [as indicated in Fig. 2(a)]. If AFCs are aligned in parallel and perpendicular to their bisecting directions, \( S \) becomes high.

A. Globally ferromagnetic order

For a small angle between the two filaments of an AFC \( (0^\circ \leq \theta_a \leq 80^\circ) \), \( R_1 \) becomes nonzero as the AFCs density increases, which indicates the globally ferromagnetic order [Fig. 2(c) and Fig. 2(a)]. \( lR_1 \) also becomes nonzero at the same density; hence, once the order emerges it grows globally, indicating phase transition [Fig. 2(c)]. Note that at \( \theta_a = 0^\circ \), an AFC is equivalent to a single polar filament, for which ferromagnetic transition was reported in earlier studies [33, 43].

Vortices and asters are not clearly distinguished in the simulation. Where the concentration of AFCs is high, directional order develops up to the system size, and defects such as vortices and asters are not observed. It is possible that they could be observed in the lower density region near the transition point; however, it is practically difficult to detect these structures at the resolution of this type of simulation. Therefore, we do not discuss vortices and asters further in the present study.

B. Moving smectic structure

Inside the region of the ferromagnetic order phase, a lamellar structure that consists of orientating AFCs is observed, as shown in Fig. 2(d). The lamellar moves in the opposite direction to that which bisects the two filaments of an AFC (see also Fig. 3 and Subsec. IV B). We call this dynamic pattern ‘moving smectic’ by analogy with the physics of liquid crystals. Although moving

FIG. 3. Color maps of the order parameters \( R_1, R_2, lR_1, \) and \( lR_2 \) on \( \theta_a \) and \( N \).

FIG. 4. Color map of the order parameters \( S \) on \( \theta_a \) and \( N \).
band structures of density wave were reported in some actively propelling systems [44, 45] (as discussed below), the smectic pattern found here is different from these because the dominant propelling direction of each particle is almost perpendicular to the band (Sec. IV). Due to the moving spatial pattern composed of aligned AFCs in parallel, the density of AFCs exhibits periodicity over time (as detected by Fourier spectrum and shown in Fig. 6). As shown in Fig. 4, order parameter $S$ distinguishes this pattern from the globally ferromagnetic order.

C. Disorder

When the density of AFCs is small, diffusion, and not the interactions among AFCs, is dominant. There is neither orientational nor spatial order. Even when the density of AFCs is high, we do not detect any sign of order in orientation, space, and time in the parameter region $80^\circ \leq \theta_a \leq 120^\circ$ [Fig. 2(e)].

D. Locally nematic order

For larger $\theta_a$ up to $180^\circ$, $lR_2$ becomes nonzero, while $R_2$ remains zero regardless of the AFCs’s density [Fig. 3(b) and (d)]. The snapshot in Fig. 2(f) clearly indicates that neighboring AFCs are aligned and bundled, whereas orientational order is not maintained at a scale larger than a few filaments length.

E. Phase diagram

A phase diagram of the system’s behavior is depicted in Fig. 7. Disorder-ferromagnetic transition is observed with small $\theta_a$, $0^\circ \leq \theta_a \leq 80^\circ$. Moving smectic structure appears in the higher density region of $30^\circ \leq \theta_a \leq 80^\circ$. As $\theta_a$ increases, these two patterns vanish and motions become disorder. For larger and obtuse angles of $\theta_a$, locally nematic orders arise in $120^\circ \leq \theta_a \leq 180^\circ$. Detailed characteristics of each pattern are summarized in Table I.

In the remainder of this paper, the number of AFCs is fixed at $N = 2,000$. The dynamics of globally ferromagnetic, moving smectic, disorder, and locally nematic patterns are analyzed by setting $\theta_a = 0^\circ, 30^\circ, 90^\circ$, and $150^\circ$, respectively (represented as stars in Fig. 7).

IV. INDIVIDUAL MOTION OF AFCS

To understand how the collective dynamics described in the preceding section are maintained, the individual motions of AFCs were studied by tracking their orbits as indicated in Fig. 8. The statistics of this motion are summarized in Fig. 9 and Fig. 10. Figure 9(b)–(e) shows histograms of positional direction ($\theta$, red) and velocity direction ($\theta_v$, green) for each AFC [Fig. 9(a)]. Here, velocity is defined by the displacement of AFCs between $\Delta t = 0.1$. Absolute velocities averaged over the AFCs in each bin are also plotted. Figure 10(b)–(e) shows histograms of the relative angle of the velocity $\theta_r$, defined in Fig. 10(a). The mean absolute value of velocity is also plotted.

FIG. 6. Fourier spectrum on a time series of AFC density at globally ferromagnetic, moving smectic, and disorder phases. Parameter values are the same as those used in Fig. 2.

FIG. 5. Time evolution of the moving smectic structure ($\theta_a = 30^\circ$ and $N = 2,000$). Two lamellas are indicated by arrow heads colored green and cyan, respectively.
A. Globally ferromagnetic order

In the parameter region of ferromagnetic order, the motion of an AFC is translational without significant rotational motion [Fig. 8(b)]. The predominant propelling direction of an AFC is perpendicular to the global orientational direction [Fig. 8(b)]. The propelling direction is also perpendicular to the positional direction as indicated in Fig. 10(b). In addition, AFCs move faster when the positional and propelling directions are perpendicular than when they are equal [Fig. 8(b) and 10(b)].

B. Moving smectic structure

In the moving smectic order, a large proportion of AFCs are aligned to form the layered bands of the lamellar structure. AFCs in the lamellar are moving along the layer [Fig. 6(c)]. As a result, in a similar but sharper manner than AFCs in the globally ferromagnetic region, the motion of individual AFCs in moving smectic is translational, and the dominant propelling direction is from the perpendicular to the positional direction [Fig. 8(c) and Fig. 10(c)]. The time span over which an AFC maintains directed motion also becomes substantially longer. At the same time, the lamellar structure itself moves slowly in the opposite direction to the bisecting direction of AFCs (Fig. 5), as represented by the finite velocity around relative angle 0° in Fig. 10(c). These behaviors are apparently contradictory to the momentum conservation that should be satisfied in the present model. Detailed analysis reveals that small parts of AFCs, which have positional and velocity directions far from the collective averages, move faster to compensate the conservation law [Fig. 8(c)].

C. Disorder

In the disorder phase, the motion is still translational, while the predominant propelling direction now coincides with its positional direction [Fig. 8(d) and Fig. 10(d)]. Because there is no orientational order, the histograms of positional direction and velocity direction are now uniform [Fig. 8(d)]. The absence of orientational order is discussed further in Subsec. VII C.

D. Locally nematic order

The motion in the locally nematic region is rotational rather than translational [Fig. 8(e)]. AFCs move at the low velocity indicated in Fig. 10(e), and are not propelled far. The alignment process of AFCs does not propagate, which results in the bundled structure of AFCs [Fig. 2(f)]. Therefore, although local alignment is strong [Fig. 3(d)], the histograms of positional and velocity directions are uniform [Fig. 8(e)].

FIG. 7. The phase diagram of the collective patterns of AFCs. (a) Globally ferromagnetic; (b) moving smectic; (c) disorder; (d) locally nematic. Precise criterion for assignment of phases in numerical simulation is based on time-averaged order parameters as follows: globally ferromagnetic: $R_1 > 0.5$ and $S < 0.55$; moving smectic: $R_1 > 0.5$ and $S > 0.55$; locally nematic: $R_1 < 0.5$ and $L^2 > 0.5$; disorder: otherwise. Stars in the figure indicate the parameters used for analyzing dynamics in the respective phases. The square indicates the parameters used in Fig. 13.

FIG. 8. Orbits of individual AFCs in the collective motion. (a) Color code of orbits. AFCs are colored along the time course from yellow to blue, and finally red. (b)–(e) Orbits of individual AFCs in the indicated phase. Ten AFCs are colored according to (a); the others are colored gray.
V. TWO-BODY INTERACTION

Investigating the interaction between AFCs is crucial for understanding the emergence of various dynamics at different parameter regions. In this section, we assess whether the completely overlapped state of two AFCs is sustained during the time evolution of the model. Linear analysis is not useful because, due to the condition that interaction works only when filaments are crossing, the state is singular. Instead, we numerically checked the stability of the overlapped state by measuring the final distance between the two initially overlapped AFCs. The distance of the two AFCs is defined by the sum of distances between the centers of L-L and R-R filaments \( d = d_L + d_R \), see Fig. 11(a), by which \( d = 0 \) corresponds to the overlapped state. The distributions of \( d \) for given values of \( \theta_a \) are evaluated by using iterating simulations. Figure 11 shows the contour map of this distribution. Eventual states are classified into six domains, (i)–(vi), corresponding to the configurations of the two AFCs depicted in Fig. 11(c). Configurations (i) and (ii) represent almost overlapped and well aligned states, where the distance \( d \) is smaller than 1, which is equal to half of the filament length \( \ell / 2 \).

In \( \theta_a < 10^\circ \), two types of configurations (i) and (iii) are possible; however, the probability of type (iii) becomes higher as \( \theta_a \) increases. For \( 30^\circ \leq \theta_a \leq 80^\circ \), there are no domains with small \( d \), indicating that the overlapped state is not maintained. In particular, configuration (iv) dominates the probability up to \( \theta_a < 20^\circ \). Where \( \theta_a \geq 80^\circ \), an almost overlapped configuration (ii) appears and the probability becomes higher as \( \theta_a \) increases, whereas the probability in non-aligned configurations becomes smaller. Within this region \( (105^\circ \leq \theta_a \leq 150^\circ) \), configuration (vi), in which two AFCs are loosely aligned, is also possible.

Figure 11(d) (red lines) shows the ratio that the eventual distance \( d \) is smaller than 1 (i.e., domains (i) and (ii)). As \( \theta_a \) increases from \( \theta_a = 0^\circ \), configurations (iii) and (iv) become more dominant and the ratio decreases to almost 0 (\( \theta_a > 10^\circ \)). The overlapped state is not stable where two AFCs move in opposite directions and are repulsive, which is responsible for the translational motions seen in globally ferromagnetic, moving smectic, and disordered states. The ratio increases with larger values of \( \theta_a \). With the disappearance of configuration (iv) where \( \theta_a > 120^\circ \), the overlapped state tends to be sustained as configuration (ii). This observation of inter-

(a)

(b) Globally ferromagnetic (\( \theta_a = 0^\circ \))

(c) Moving smectic (\( \theta_a = 30^\circ \))

(d) Disorder (\( \theta_a = 90^\circ \))

(e) Locally nematic (\( \theta_a = 150^\circ \))

FIG. 9. Statistics of positional and velocity directions. (a) Explanation of positional and velocity directions (\( \theta \) and \( \theta_v \)) for an AFC. (b)–(d) The frequencies of positional and velocity direction are shown in red and green, respectively. Points indicate the mean magnitude of velocity averaged in each bin.

(a)

(b) Globally ferromagnetic (\( \theta_a = 0^\circ \))

(c) Moving smectic (\( \theta_a = 30^\circ \))

(d) Disorder (\( \theta_a = 90^\circ \))

(e) Locally nematic (\( \theta_a = 180^\circ \))

FIG. 10. Statistics of relative angle \( \theta_r \). (a) Relative angle \( \theta_r \) is defined by the propelling direction of an AFC and its positional direction in the past. (b)–(e) Frequencies of relative angle in the four phases are shown in histograms. Plotted points represent the average magnitudes of the AFCs' velocity in each bin.
action between two AFCs is critical for the local nematic pattern, in which translational motion is suppressed and AFCs are well aligned.

VI. CROSSING OF AFCS AND FILAMENTS

In this section, we investigate how AFCs in a population of AFCs cross with each other to achieve characteristic patterns dependent on parameters. In particular, because only the angle between crossing filaments determines the development of an AFCs position in Eq. (3), our main interest is the relative angle distributions among interacting AFCs. Two types of angle are measured below. The first is the angular difference between crossing filaments, $\theta_s$, as shown in Fig. 12(a). The second is the angular difference between AFCs, $\theta_c$, measured between bisecting directions of contacting AFCs [Fig. 12(b)].

Because an AFC has two filaments, complexity arises from the variety of crossing combinations for each filament. By ignoring double crossings, we classify crossings into four types, namely RR, LR, RL, and LL, which are depicted schematically in Fig. 13(a). Frequencies of these crossing are shown in Fig. 13(b).

A. Crossing of single active filaments

First, we investigate crossing in a single active filament system ($\theta_a = 0^\circ$). In this case, $\theta_s$ is equal to $\theta_c$. Distributions of the angles are dependent on the density $\rho$ [Fig. 12(d)]. Despite the global order ($N = 2,000$), individual alignments of contacting filaments are not perfect, i.e., the crossing pair usually separates before they are fully aligned. Accordingly the angular distribution, $P(\theta_s)$, is not highest at $\theta_s = 0^\circ$ [Fig. 12(d)]. The mean and standard deviation of the angular difference, i.e., $\mu$ and $\sigma$, are calculated from the distribution of $|\theta_s|$ to be $\mu = 66^\circ$ and $\sigma = 39^\circ$, respectively.
B. Moving smectic structure

In Fig. 12(e), the green line shows the distribution of the angle between filaments, \( P(\theta_a) \), in the moving smectic phase. Compared with the ferromagnetic order phase, the angular difference between AFCs is smaller \((\mu = 56^\circ)\) and is more sharply distributed \((\sigma = 31^\circ)\). In addition, in the moving smectic phase, frequencies of crossing types R-L and L-R are significantly higher than those of the other types [Fig. 13(b)]. By considering the superposition of the shape angle of an AFC, \( \theta_a \), and the angular difference between crossing filaments, \( \theta_s \), the perfect alignment between contacting pairs of AFCs can be explained, as indicated by the distribution of \( \theta_c \) [Fig. 12(e), red line] where \( P(\theta_c) \) is highest at \( \theta_c = 0^\circ \). As a result, alignment of AFCs proceeds along the perpendicular direction to the bisecting direction, resulting in the lamellar structure.

C. Disorder

The angle between crossing filaments, \( \theta_s \), is most frequently found in the perpendicular direction. This distribution is almost identical to those observed for collections of single filaments with random orientation. Consistently, both the distribution of \( \theta_c \) [Fig. 12(f), red line] and crossing types [Fig. 13(b)] are almost uniform. These results indicate that orientational order does not exist, not even locally.

D. Alignment in the locally nematic phase

In the locally nematic phase, local alignment processes make AFCs overlap and form a bundle structure. In the bundle, the alignment is almost perfect as indicated by a sharp peak in the distribution of angular differences of AFCs at \( \theta_c = 0^\circ \) [Fig. 12(g), red line]. In the distribution of angular differences in crossing filaments, several peaks appear [Fig. 12(g), green line]. These peaks can be explained by interactions of two AFCs, as shown in Fig. 11(b) and (c). The peaks at \( \theta_s = 0^\circ \) are due to LL/RR crossings corresponding to configuration (ii), whereas the peaks at \( \theta_s = \pm \theta_a \) are due to LR/RL crossings corresponding to configuration (iii). The other two peaks in the neighbors of \( \theta_s = 0^\circ \) are produced by configuration (vi).

E. Fitting \( \theta_c \) distributions by \( \theta_s \)

Aside from the constraint to keep the shape of an AFC, each filament obeys the same equations that are independent of \( \theta_s \). Therefore, once we know how single filaments cross each other, we could also explain how AFCs cross each other by superposing alignments of the two filaments on an AFC. To test this possibility, we performed fitting of the angular distributions in \( \theta_c \) with those in \( \theta_s \). If the crossing angle of single filaments is in RR or LL, the contributions to the distributions in \( \theta_s \) and \( \theta_c \) are coincident. Conversely, if the crossing angle is in RL or LR, the contribution to \( P(\theta_c) \) is shifted from \( \theta_s \) to \( \theta_c = \theta_s \pm \theta_a \). Thus, we superpose \( P(\theta_c) \) and \( P(\theta_s \pm \theta_a) \) depending on the ratio of crossing types [Fig. 12(c) and Fig. 13].

The fittings [Fig. 12(e)–(g), broken lines] are successful in the disorder and the locally nematic patterns where \( P(\theta_c) \) can be predicted. This implies that two-body angle correlation is sufficient for understanding the structure of these patterns. In contrast, in the moving smectic pattern the actual distribution of \( \theta_c \) has a sharper peak at \( \theta_c = 0^\circ \) than those predicted by the fitting, indicating that higher-order spatial correlation is involved in achieving perfect alignment of AFCs.

VII. HEAVY-ANCHOR MODEL

We have hitherto investigated the case that an anchor of an AFC has a much smaller mass than the filaments. Here, we briefly evaluate a scenario where the anchor is much heavier and the center of inertia is at the minus end, and we provide results accordingly. In the heavy-anchor model, the equation with respect to \( \dot{\theta}_{i,k} \) is replaced by

\[
\dot{\theta}_{i,k} = \frac{T_m}{\pi \zeta_{\text{rot}} \sigma} \left[ (R_{ka,ia} - R_{ia,ka})_x (U_{k,i})_y - (R_{ka,ia} - R_{ia,ka})_y (U_{k,i})_x \right],
\]

where \( R_{ia,ka} \) is the position of the \( i(k) \)-th filament’s anchor.

Different patterns of AFCs appear in the model, especially with acute \( \theta_a \). Some snapshots are depicted in Fig. 14. For angles that are exceedingly small, where \( \theta_a \approx 5^\circ \), a ray-like aster structure is formed [Fig. 13(a)]. As \( \theta_a \) increases to \( \approx 15^\circ \), a globally ferromagnetic pattern emerges [Fig. 13(b)]. Where \( \theta_a \approx 30^\circ \), a lamellar structure composed of aligned AFCs appears [Fig. 14(c)]. In contrast to the moving smectic phase in the light-anchor model, the lamellar is winding and exhibits strong curvature. In general, the pattern arising in the heavy-

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**FIG. 13.** Crossing types of AFCs. (a) An example of a crossing type. In the image, filaments cross at RL. (b) Frequencies of crossing types for the four patterns.
TABLE I. Summary of emergent patterns (the light-anchor model).

| Patterns | Globally ferromagnetic | Moving smectic | Disorder | Locally nematic |
|----------|------------------------|----------------|----------|-----------------|
| \( \theta_a \) | \(0^\circ - 80^\circ\) | \(30^\circ - 80^\circ\) | \(80^\circ - 120^\circ\) | \(120^\circ - 180^\circ\) |
| Density transition | \(\times\) | \(\times\) | \(\times\) | \(\times\) |
| Characteristic movement | Translational perpendicularly to AFC | Translational perpendicularly to AFC | Translational parallel to AFC | Rotational |
| Alignment between crossed AFC’s | Imperfect | Perfect | None | Strong 2-times symmetry |
| Alignment propagation | Isotropic | Perpendicular to AFC | None | None |

anchor model is less dynamic than that in the light-anchor model.

There are two possible reasons why the emergent patterns in the heavy-anchor model are so different from those in the light-anchor model. The first reason is the difference in how filaments can cross. In the heavy-anchor model, the tendency towards alignment of AFCs is stronger. By using the same analysis of two AFCs performed in Sec. V, the distributions of \(d\) shown in Fig. 15 are obtained for the heavy-anchor model. Compared with Fig. 11, the contour is simpler; there are only two configurations and domains with large \(d\) do not exist where \(\theta_a\) is small. Additionally, the ratio of \(d < 1\) is larger than in the light-anchor model shown in \(0^\circ \leq \theta_a \leq 30^\circ\) [Fig. 11(b)]. Consistently, alignment of two single filaments \((\theta_a = 0^\circ)\) in a population is perfect, as shown in Fig. 11(a) where \(P(\theta_a)\) has a sharp peak at \(\theta_a = 0^\circ\) \((\mu = 7^\circ\) and \(\sigma = 25^\circ\)).

The second reason is the velocity of each AFC. Because a high probability with small \(d\) implies that a less repulsive force exists between two AFCs, the individual motion of AFCs is more suppressed in the heavy-anchor model, whereas the preferred propelling direction is not drastically changed [Fig. 11(b)]. Therefore, in contrast to the light-anchor model, the alignment process is localized and does not propagate far; hence, defects such as ray-like aster structures can survive and are maintained.

In the majority of previous studies, objects with simpler shapes, such as material points, spheres, rods, or ellipsoids, whether stiff or flexible, were assessed.\(^{21,22}\) Shapes that are more complex, however, can play important roles in biological systems. For example, self-organization of microtubules ~10 nm beneath the apical membrane of multi-ciliated cells is associated with regular configuration of cilia.\(^{38,39}\) With the aim of understanding the dynamics of molecular complexes of active filaments, we performed two-dimensional simulations of interacting AFCs, defined as connected pairs of biofilaments, whose shape was characterized by the angle between the two filaments.

AFCs exhibited several types of collective patterns with global and local orders. The moving smectic order is especially interesting because it emerges by mechanisms that have not previously been reported.\(^{44,45}\) For example, Head et al.\(^{55}\) reported a moving band structure composed of aligned filaments in parallel. Although their structures look similar, the individual motions of the filaments are strikingly different in the model of Head et al.

FIG. 15. Two-body interaction in the heavy-anchor model. (a) Frequency of \(d\) on \(\theta_a\) in the heavy-anchor model, which is comparable to Fig. 11(b). (b) Characteristic configurations for each domain are depicted in (i’) and (ii).

(a) Ray-like aster \((\theta_0 = 5^\circ, N = 3000)\) (b) Globally ferromagnetic \((\theta_0 = 15^\circ, N = 3000)\) (c) Smectic \((\theta_0 = 30^\circ, N = 3000)\)

FIG. 14. Snapshots of simulation results in the heavy-anchor model. Each filament is colored in the same manner as Fig. 4 (a)–(c) Patterns are shown with indicated parameter values.
compared to those in the model presented here; specifically, the moving direction of the individual filaments coincides with that of the band. The mechanism we observed for formation of the structure is also distinct from earlier studies, where the filaments self-propel and momentum is not conserved (such systems are classified as ‘active dry systems’ in [23]). In the present model, the translational motion required for emergence of orders (see below) is maintained by the interaction among AFCs.

The causes of emergent patterns can be understood by tracing the orbits of AFCs and investigating the alignment between crossing pairs of AFCs, as described in Sec. IV, Sec. V, and Sec. VI. Analysis of two-body interaction revealed that the overlapped state of AFCs was maintained where \( \theta_0 \) was large, which was responsible for appearance of the local nematic order. In contrast, instability of the overlapped state indicates repulsion between the two AFCs, which is required for translational motion. If AFCs move translationally and the alignment process can propagate, ferromagnetic orders can grow over a range that is much longer than filament length. In the moving smectic phase, the individual motion of AFCs is constrained in a direction perpendicular to the AFCs’ bisector and, thus, a lamellar structure is formed. The translational motion may be necessary for establishing the global orders because phase transition of continuous order parameters in a two-dimensional system is possible only when long-range interaction is present [46]. Employing continuum description [40, 47] will be useful for investigating the stability of these patterns.

We also studied the heavy-anchor model, i.e., the case in which the mass of the anchor is much heavier than that of the filaments. The emergent patterns from the heavy-anchor model, including ray-like asters, were different from those of the light-anchor model due to the stronger tendency towards complete alignment of the two single crossed filaments and the slower motion of the action.

The present study ignored some potentially important interactions for modeling experimental situations. For example, it is possible that the length of filaments and the shape of AFCs are not uniform and change during the time evolution. In particular, active regulation of filament length can be important for establishing ordered patterns, as exemplified by microtubule-bundles in plant cells. Furthermore, excluding volume effect can result in alignment of the filaments and appearance of nematic order [27–31]. All of these processes can contribute to the organization of biofilament networks in actual systems. In further research, the present analyses for AFCs could be easily extended, and this would likely provide useful insights for understanding collective patterns in more complex scenarios including the aforementioned processes. The rapid development in bio-nano engineering will also enable a comparison between experimental systems and those that are simulated.

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**FIG. 16.** Statistics from the heavy-anchor model. (a) Distribution of \( \theta_0 \) at \( \theta_0 = 0^\circ \), comparable to Fig. (d). (b) Histogram of relative angle \( \theta_0 \) at \( \theta_0 = 0^\circ \), comparable to Fig. (d). Mean absolute velocity in each bin is also plotted.
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