“Inchworm Filaments”: Motility and Pattern Formation

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Abstract

In a previous paper, we examined a class of possible conformations for helically patterned filaments in contact with a bonding surface. In particular, we investigated geometries where contact between the pattern and the surface was improved through a periodic twisting and lifting of the filament. A consequence of this lifting is that the total length of the filament projected onto the surface decreases after bonding. When the bonding character of the surface is actuated, this phenomenon can lead to both lifelike “inchworm” behavior of the filaments and ensemble movement. We illustrate, through simulation, how pattern formation may be achieved through this mechanism.

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I. INTRODUCTION

In previous work[1], we explored a toy model for the Amyloid beta fibril CF-PT and a class of conformations for that model which lead to large bonding energies when in contact with a flat surface. Motivated by the proposition that CF-PT (cylindrical filament with periodic thinning) is a precursor filament for PHF (paired helical filament)[2], we showed that one such strongly bonded conformation for our model is a helix like that of PHF. This earlier investigation was limited to a surface with a static, uniform bonding energy. Here we consider the possibility of a flat, nonbonding surface with a moving bonding region and discuss the dynamic conformational change and translation of the filament associated with moving the region beneath it. To clarify, we do not consider the case where the surface itself is moving but rather that the region of the surface which has the potential to bond with the filament varies in time (due to electrical charge, chemical variation, etc.). As in the previous study, we consider a “close contact” approximation for the nature of the bonding between the surface and the filament; that is, the bonding energy between a point on the filament and a point on the surface is nonzero only if these two points are in contact.

Our model filament consists of a cylinder with a helical bonding pattern, of period $L$, such that only the patterned region of the filament may bond with the surface. We will refer to a segment of the filament of length $L$ where the bonding pattern is in contact with the surface at the beginning and end of the segment as a “monomer”. A cartoon of two monomers is shown below in Figure 1 A. To assume the helical conformation, each monomer twists to align the bonding pattern with the surface at both ends, and bends in the center. A sketch of a monomer in the helical conformation is shown below in Figure 1 B. A consequence of this bending is that the monomer lifts off the surface in the center and the length of the monomer projected onto the surface decreases by some amount $\Delta L_{\text{Bond}}$. This is illustrated in Figure 1 C, and a cartoon of a filament comprising three monomers assuming the helical conformation is displayed in Figure 1 D, shown below.
II. SIMULATION

With the conformational change discussed above in the presence of a bonding surface, we know that if we can actuate the surface in such a way that the bonding character changes with time, we can control the filament shape as well. Furthermore, we can show that with the right actuation, the filament is subject to not only a temporary shape change while bonded, but a net displacement. Thus with continued surface actuation, filament motility and “migration” can be achieved.

This displacement stems from an asymmetric shortening and lengthening of the filament when a bonding region is introduced and removed. When the filament binds to the surface, each monomer curls up, as shown above, decreasing the contact length by an amount $\Delta L_{\text{bond}}$ and moving the endpoints of the whole filament inwards. Similarly, when the filament
unbinds, each monomer stretches out, moving the endpoints outwards. If the bonding region is brought in contact with and removed from the entire filament simultaneously, this movement of the endpoints is symmetric and the filament faces no net displacement; however, if a bonding surface is present beneath one end of the filament and not the other, the motion of the bonded end can be expected to be more restricted than that of the unbonded end (due to increased friction with the surface etc.). This leads to filament motion contrary to the motion of the bonding region. As the bonding region is introduced, the filament preferentially shortens from the unbonded end moving towards the oncoming bonding section. As the bonding region is removed, the filament preferentially lengthens away from its direction of retraction. This motion qualitatively resembles that of an inchworm.

When simulating motion due to surface actuation, we need to approximate how motion of bonded monomers is restricted compared to that of non-bonded monomers. In reality this will widely vary based on both the filament and surface materials but for the purposes of constructing an illustrative simulation, we will assume the following conditions. 1) each bound monomer confers the same restriction to motion when bound and 2) in the limit where only one monomer is unbound, only the unbound monomer moves. Now let $N$ be the total number of monomers in the filament, $n$ be the number of those bonded, for illustrative purposes assume a large $\Delta L_{\text{Bond}}$ of $\frac{L}{2}$, and denote $\mathbf{p}(1)$ and $\mathbf{p}(N)$ as the positions of the first and last monomers respectively. We may now consider the displacement of the monomer at $\mathbf{p}(1)$ in the direction of $\mathbf{p}(N) - \mathbf{p}(1)$.

$$
\text{Displacement of } \mathbf{p}(1) = \begin{cases} 
\text{contracting} & \begin{cases} 
\text{only } \mathbf{p}(1) \text{ is bound} \quad \frac{L}{4} \left(1 - \frac{n}{N}\right) \\
\text{only } \mathbf{p}(N) \text{ is bound} \quad \frac{L}{4} \left(1 + \frac{n}{N}\right) \\
\text{else} \quad \frac{L}{4} 
\end{cases} \\
\text{extending} & \begin{cases} 
\text{only } \mathbf{p}(1) \text{ is bound} \quad -\frac{L}{4} \left(1 - \frac{n}{N}\right) \\
\text{only } \mathbf{p}(N) \text{ is bound} \quad -\frac{L}{4} \left(1 + \frac{n}{N}\right) \\
\text{else} \quad \frac{L}{4} 
\end{cases}
\end{cases}
$$

(1)

Using this displacement rule, we may propagate the position of the filament as we move the bonding region. Motion of a single filament with a rightward moving, green bonding region is shown below in Figure 2.
Figure 2: Leftward filament migration (time progresses from left to right and top to bottom) in response to a rightward moving, green bonding section.

We may note that filaments will self-order by length (see Figure 3, Sub-Figure a, below) as with each pass of the bonding region, a longer filament experiences a greater translation (due to a larger number of monomers).

Filament translation in 2D can be achieved by introducing motion of the bonding region along two perpendicular axes. In this case, the shift of a filament caused by motion along one axis can oppose that from the other in part or in full resulting in reduced or null motion for filaments of the proper orientation. In the simulation displayed in Figure 3, Sub-Figure b, the bonding region moves from left to right and bottom to top. If a filament is oriented such that the angle its tangent axis makes with the $x$-axis is $\frac{3\pi}{4}$ or $\frac{7\pi}{4}$, the motion resultant from the vertical bonding actuation completely cancels that from the horizontal and the filament does not move. Orientations corresponding to angles from $\frac{\pi}{2}$ to $\pi$ and $\frac{3\pi}{2}$ to $2\pi$ experience a similar reduction in motion.
(a) Self ordering of filaments by length: as time progresses from left to right, longer filaments move farther.

(b) 2D translation (Time progresses from left to right.): the bonding region moves from left to right and bottom to top. If a filament is oriented such that the angle its tangent axis makes with the $x$-axis is $\frac{3\pi}{4}$ or $\frac{7\pi}{4}$, the motion resultant from the vertical bonding actuation completely cancels that from the lateral and the filament does not move (top left filament). To contrast, a filament oriented such that the angle its tangent axis makes with the $x$-axis is $\frac{5\pi}{4}$ or $\frac{9\pi}{4}$ benefits from maximum translation (bottom left filament). Filaments aligned with either axis move only along that axis.

Figure 3: Self organization of filaments by length and 2D translation.

When many filaments with different orientations are introduced to a bonding region which moves along two perpendicular axes, as described above, ring formation occurs. Filaments “migrate” with a direction and magnitude dependent on the angle their tangent axes make with the $x$-axis.
III. DISCUSSION

We’ve shown that when in contact with a time-varying attractive surface, helically-patterned filaments may self-sort by length and orientation. When many of these filaments are placed on such a surface, they can self-assemble into rings. We hope that this mechanism has potential applications in the self-organization of materials. Additionally, the phenomena discussed in this work may have some pathological relevance in explaining the aggregation of proteins. Many diseases are characterized by protein disorganization and aggregation e.g. Amyotrophic Lateral Sclerosis[3] and other neurodegenerative pathologies[4] though this mechanism is unlikely to have any physiological relevance, perhaps the idea of surface-mediated filament migration has some merit. The filament migration described above, if observed in a bounded region, would result in aggregation at the boundaries and stochastic surfaces charges seen in biological systems may resemble the surface actuation described above.

IV. REFERENCES

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