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Modeling of rate-dependent phase transition in bacterial flagellar filament

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ABSTRACT

Recent experiment of Darnton and Berg [34] showed that phase transition of bacterial flagellar filament is loading rate-dependent. The object of this paper is to describe the observed loading rate-dependent phase transition responses of the filament by using time dependent Ginzberg–Landau continuum model. We developed a finite element method (FEM) code to simulate the phase transition under a displacement-controlled loading condition (controlled helix-twist) by using viscosity-type kinetics. Our FEM simulation captures the main features of the rate-dependence: under slow loading (i.e., loading time $\gg$ the relaxation time) the filament phase transition is an equilibrium process and each phase grows via interface propagation on the Maxwell line; under rapid loading (i.e., loading time $\ll$ the relaxation time), the phase transition does not occur and the response is elastic. Our FEM model provides a tool to study the effects of loading-rate dependent phase transition for bio-filament with viscous kinetics.

1. Introduction

The motion of the flagella of live bacteria was first observed by Ehrenberg [1] in 1838. Flagella-based motility is a major mode of locomotion for bacteria. The long helical filament is the propeller made up of only one kind of protein called flagellin [2,3]. Macroscopically the filament can be viewed as a hollow tube with an outer diameter of 20 nm and a length of 15–20 μm and can take a helical shape [4]. As shown in Fig. 1(a) and (b), when the bacterium swims, the flagella form a rotating bundle as the motor is in counter clockwise (CCW) rotation. When the motor rotation reverses, transition from normal (*N*) phase to semi-coiled (*SC*) phase occurs in the filament [5–8]. A filament has 12 phases with different radii and pitch lengths, whose microstructure difference is characterized by the protein subunit misfit (e.g., 0.8 Å). The transition of the filament from one phase to another can be induced by chemical change or by mechanical loading [9–16,34]. The mechanical analysis on the experiment of Hotani [17] showed that both torque and bending moment contribute to the new phase nucleation, and they are near zero at the interface (phase front) during the equilibrium phase growth. This is consistent with the thermodynamic equilibrium phase transition condition: Maxwell forces are zero and the two coexisting phases have the same free energy [17]. Berg's recent experiment [34] showed that the phase transition of filament is loading rate-dependent, as shown in Fig. 2 where filament undergoes phase transition between normal and hyperextended form by pulling. Under rapid pulling (0.4 μm/s), the filament usually traces a simple elastic, hysteresis-free curve, and often (9 of 19 cycles) consists a complete elastic extension–compression cycle without experiencing a polymorphic transformation. When the filament is extended much more slowly (0.04 μm/s), it always transforms (10 of 10 cycles), and the transformation generally occurs at lower force levels (Fig. 2, inset). Our object of this paper is to describe the loading rate-dependent phase transition of bacterial flagellar filament by using Time dependent Ginzburg–Landau continuum model and FEM simulation.

In the literature, there are several theoretical models proposed to describe the phase transition behavior of flagellar. Goldstein et al. [18] and Coombs et al. [19] proposed the bistable energy function to represent two equilibrium phases, and qualitatively explained the chirality transition of a filament observed in Hotani's experiment. Power et al. [20,21] proposed another continuum theory for the polymorphism of the filament to account for the alternate stable conformations. Stark et al. [35,36] presented a coarse-grained model for the filament by introducing an elastic network of rigid bodies and using Ising Hamiltonian to address the two states of the flagellin protein. Wada et al. [37] introduced a bistable helical filament model that accounts for different elastic monomeric states by a discrete Ising-like spin variable along the arclength. By hybrid Brownian dynamics Monte–Carlo simulations, Wada et al. [37] showed that filament phase transition is pulling rate dependent. In modeling the observed phase transition

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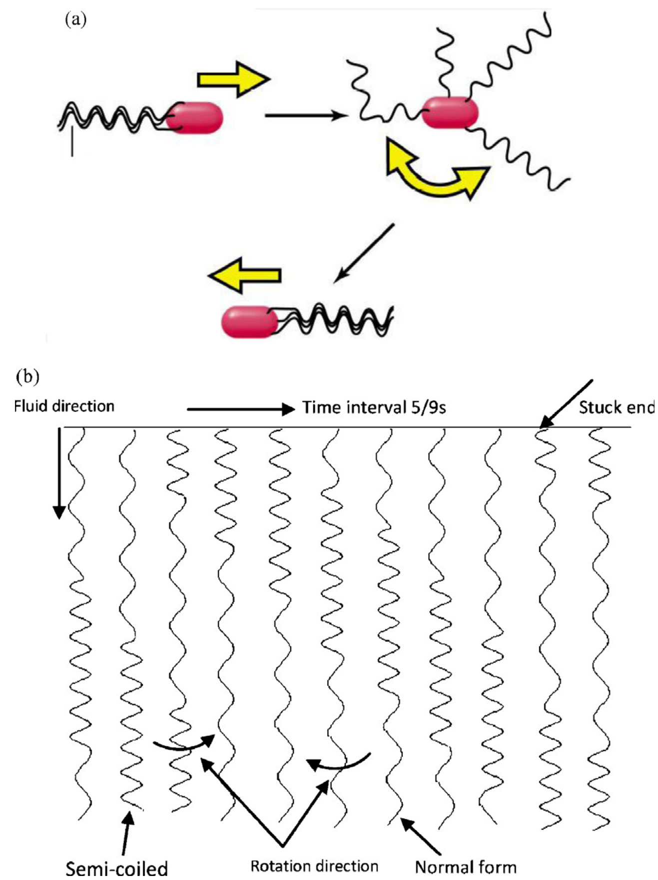

Fig. 1. (a) Illustration of movements of *Escherichia coli*, when its motor rotates CCW, flagella are in a bundle and the cell swims; when the motor reverses direction, flagella fall apart and the cell tumbles. (b) Transition between normal and semi-coiled form under external viscous fluid force.

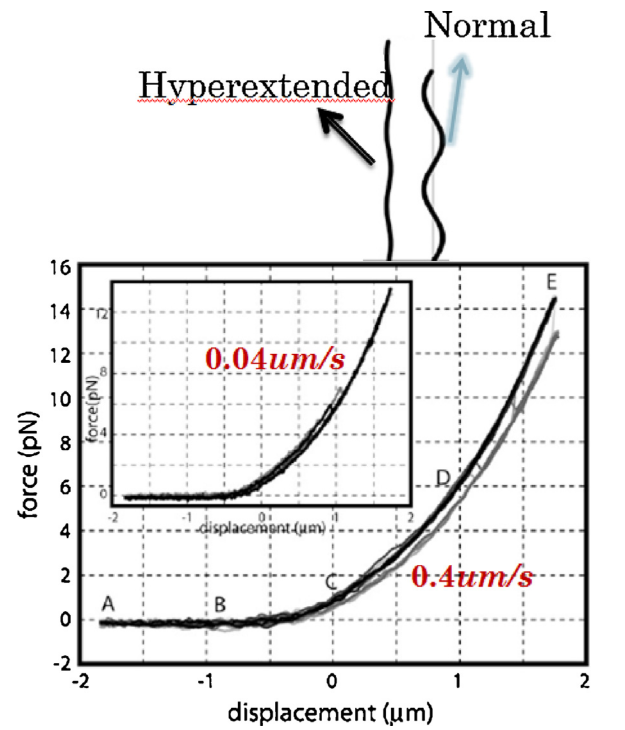

Fig. 2. Filament pulling experiment of Berg [34]. Force–extension curves for pulling on a normal ($n = 2$) polymorphic form filament. It shows 10 force–extension measurements performed at an extension rate of 0.4 um/s. During 6 of the 10 trials shown, the filament followed a simple elastic force–extension curve (labeled A–E). During the other trials a polymorphic transformation to the hyperextended ($n = 1$) form occurred during the extension of the filament, dropping the force onto a lower curve. When the same filament was pulled at a 10-fold slower extension rate, it transformed during every trial (inset) at about half of the force required during rapid pulling. The flat near-zero portion corresponds to filament buckling (A and B). Trap stiffness was 90 pN/mm. The location of zero displacement is arbitrary.

kinetics and the rate dependent responses, the time dependent Ginzberg–Landau continuum model could be a good model candidate and can be implemented into FEM simulation to quantify filament phase transition behavior. Moreover, in order to describe the phase transition process, such as phase nucleation and growth with interface propagation, a non-local formulation of interfacial energy need to be included, similar to the simulations of the localized deformation in the phase transition process of many shape memory alloys [22,23].

In this paper, we introduce a theoretical framework of the time dependent Ginzberg–Landau viscoelasticity and implement it in a 1D non-local finite element method (FEM) code to simulate the filament's phase transition phenomena and to describe the observed loading rate dependent effects. The theoretical framework and the FEM implementation are introduced in Sections 2 and 3, respectively. In Section 4, the results of the FEM simulation are discussed. Summary and conclusions are given in Section 5.

2. Non-convex non-local viscoelasticity

The Lagrange formulation for non-local viscoelasticity [22–25] is:

$$\frac{\delta U}{\delta q_i} + \frac{\delta D}{\delta \dot{q}_i} = 0 \tag{1}$$

where $U = \int(W + G)dx$, $D = \int R dx$,x is the spatial coordinate of the 1D model; δq_i and $\delta \dot{q}_i$ represent the variations of the freedom and the rate of the freedom ($\delta \dot{q}_i = \delta(dq_i/dt)$), respectively. W, G and R are respectively the nonconvex elastic energy density, that describes material instability and phase transition [26–28], the nonlocal gradient energy density to account for the interfacial energy [26–29], and the Rayleigh dissipation function for the viscous overdamping kinetics [22,23,25]. To use the framework to describe the flagella phase transition, suitable energy formulations for the flagella – non-convex elastic energy, elastic gradient energy and dissipation energy – are needed.

2.1. Non-convex elastic energy

A Landau free energy (non-convex) is used to describe the elastic energy of the filament. The equilibrium twist and curvature of the N phase and SC phase of the filament are (−2, 1.2) and (2, 2.4) respectively (unit: rad/μm). For simplicity, we consider only the twist difference of the two phases in the energy formulation. That means, the non-convex elastic energy is a function of the twist. For mathematical convenience, we shift the equilibrium twist from (−2, 2) to (0, 4), and express the elastic energy density as

$$W = 16 \times 10^{-25}\gamma^2 - 8 \times 10^{-25}\gamma^3 + 1 \times 10^{-25}\gamma^4 \tag{2}$$

where γ denotes the twist (per unit length). Eq. (2) is plotted in Fig. 3(a), which has two equilibrium phases.

2.2. Non-local gradient energy

To describe the energy of the interface between the coexisting phases, non-local energy (gradient energy) density [26,28] is included in the current model.

$$G = g \cdot (\gamma')^2 \tag{3}$$