Simulation of bacterial flagellar phase transition by non-convex and non-local continuum modeling

Xiaoling Wang, Yongjun He, and Qingping Sun

1) School of Mechanical Engineering, University of Science and Technology Beijing, Beijing 100083, China
2) UME-MS, ENSTA-ParisTech, Chemin de la Hunière, 91761 Palaiseau Cedex, France
3) Department of Mechanical Engineering, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China

(Received 06 April 2011; accepted 14 May 2011; published online 10 July 2011)

Abstract Bacterial flagellar filament can undergo a stress-induced polymorphic phase transition in both vitro and vivo environments. The filament has 12 different helical forms (phases) characterized by different pitch lengths and helix radii. When subjected to the frictional force of flowing fluid, the filament changes between a left-handed normal phase and a right-handed semi-coiled phase via phase nucleation and growth. This paper develops non-local finite element method (FEM) to simulate the phase transition under a displacement-controlled loading condition (controlled helix-twist). The FEM formulation is based on the Ginzburg-Landau theory using a one-dimensional non-convex and non-local continuum model. To describe the processes of the phase nucleation and growth, viscosity-type kinetics is also used. The non-local FEM simulation captures the main features of the phase transition: two-phase coexistence with an interface of finite thickness, phase nucleation and growth with interface propagation. The non-local FEM model provides a tool to study the effects of the interfacial energy/thickness and loading conditions on the phase transition. © 2011 The Chinese Society of Theoretical and Applied Mechanics. [doi:10.1063/2.1104401]

Keywords polymorphic phase transition, bacterial flagellar filament, Ginzburg-Landau, non-local elasticity, finite element method, non-convex viscoelasticity

The motion of the flagella of live bacteria was first observed by Ehrenberg 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. 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. As shown in Figs. 1(a) and 1(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. 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 × 10^{-10} nm). The phase transition of the filament can be induced by chemical change or by mechanical loading. The mechanical analysis on the experiment of Hotani showed that both torque and bending moment contribute to the phase nucleation, and they are close to 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.

In literatures, there are several theoretical models proposed to describe the phase transition behavior of flagellar. Goldstein et al. and Coombs et al. proposed a 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. proposed another continuum theory for the polymorphism of the filament to account for the alternate stable conformations. Since the constitutive models of the filament are strong non-linear, exact analytical solutions are difficult to obtain. 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. So far, there is no simulation tool capable of describing the bacterial flagella phase transition.

In this paper, we introduce a theoretical framework of the non-convex non-local viscoelasticity and implement it in a one dimensional (1D) non-local finite element method (FEM) code to simulate the filament’s phase transition. The theoretical framework and the FEM implementation are introduced later, the results of the FEM simulation are discussed and summary and conclusions are given.

The Lagrange formulation for non-local viscoelast-
\[ \frac{\delta U}{\delta \gamma_i} + \frac{\delta D}{\delta \dot{\gamma}_i} = 0, \quad (1) \]

where \( U = \int (W + G) \, dx \), \( D = \int R \, dx \); \( x \) is the spatial coordinate of the 1D model; \( \delta \gamma_i \) and \( \delta \dot{\gamma}_i \) represent the variations of the freedom and the rate of the freedom (\( \delta \dot{\gamma}_i = \delta (d\gamma_i/dt) \)), respectively; \( W \), \( G \) and \( R \) are respectively the nonconvex elastic energy density which describes material instability and phase transition, the nonlocal gradient energy density to account for the interfacial energy, and the Rayleigh dissipation function for the viscous overdamping kinetics. 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.

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 \((2, 2.4)\) (unit: rad/\(\mu m\)). 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

\[ W = 16 \times 10^{-25} \gamma^2 - 8 \times 10^{-25} \gamma^3 + 1 \times 10^{-25} \gamma^4, \quad (2) \]

where \( \gamma \) denotes the twist (per unit length). Equation (2) is plotted in Fig. 2, which has two equilibrium phases.

\[ G = g \cdot (\gamma')^2, \quad (3) \]

where \( \gamma' = d\gamma/dx \) and \( g \) contains a material intrinsic length characterizing the interface thickness.

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

\[ R(\dot{\gamma}) = 16 \times 10^{-25} \dot{\gamma}^2 t_r, \quad (4) \]

where \( t_r \) is the material characteristic relaxation time, the unit of \( W \), \( G \) and \( R \) is Nm. It is noted that the dissipative energy function is positive definite.

The procedures for implementing the non-convex non-local viscoelasticity model in FEM simulation are reported.

To calculate the integration of the free energy along the filament (\( x \) coordinate) in Eq. (1), the filament is discretized into elements. The displacement field (distribution of the torsion angle) in the element is represented by the nodal displacements and proper shape functions. In the present FEM model, the nodal displacement is the torsion angle; the derivative of the displacement is the twist. As shown in Eqs. (1) and (3), the energy of the system includes both the twist and the twist gradient. So, elements with C-1 continuity are used in the current model.

In Fig. 3, the filament (length 20 \( \mu m \)) is divided into \( n - 1 \) elements with \( n \) nodes. Each element has two nodes and each node has two nodal degrees of freedom:
where the shape functions are
\[\theta = [h_1 \ h_2 \ h_3 \ h_4] \times \begin{bmatrix} \theta_i \\ \theta_{i,x} \\ \theta_{i+1} \\ \theta_{i+1,x} \end{bmatrix}, \quad (5)\]

where the shape functions are
\[h_1 = \frac{1}{4} (1 - m)^2 (2 + m), \quad h_2 = \frac{h}{8} (1 - m^2) (1 - m), \quad h_3 = \frac{1}{4} (1 + m)^2 (2 - m), \quad h_4 = \frac{h}{8} (-1 + m^2) (1 + m).\]

Fig. 3. Nodal freedoms and elements used in the FEM simulation. The filament is divided into \(n - 1\) elements; each element has two nodal freedoms: \(\theta, \theta_{,x}\); \(h\) is the element length.

Here \(m\) is the local coordinate of an element; and the local coordinates of the two nodes in one element is \(-1\) and \(1\), respectively (Fig. 3). With the displacement field (torsion angle field) in Eq. (5), the twist \(\gamma\) and twist gradient \(\gamma'\) can be expressed as
\[\gamma = \left[\frac{\partial h_1}{\partial x} \ \frac{\partial h_2}{\partial x} \ \frac{\partial h_3}{\partial x} \ \frac{\partial h_4}{\partial x}\right] \times \begin{bmatrix} \theta_i \\ \theta_{i,x} \\ \theta_{i+1} \\ \theta_{i+1,x} \end{bmatrix}, \quad (6)\]
\[\gamma' = \left[\frac{\partial^2 h_1}{\partial x^2} \ \frac{\partial^2 h_2}{\partial x^2} \ \frac{\partial^2 h_3}{\partial x^2} \ \frac{\partial^2 h_4}{\partial x^2}\right] \times \begin{bmatrix} \theta_i \\ \theta_{i,x} \\ \theta_{i+1} \\ \theta_{i+1,x} \end{bmatrix}. \quad (7)\]

Substituting Eqs. (6), (7) and (2)–(4) into the energy variation Eq. (1) and assembling all the elements, we can obtain\(^{23,50}\) the equilibrium equations as
\[\tilde{K} \cdot \ddot{q} + \tilde{C} \cdot \dot{\ddot{q}} = 0, \quad (8)\]

where \(\ddot{q}\) is a vector containing all the nodal freedoms of the system; \(\tilde{K}\) and \(\tilde{C}\) are the stiffness and viscosity matrices, respectively. Since the material constitutive energy is non-linear (non-convex elastic energy in Eq. (2)), \(\tilde{K}\) is not a constant matrix, but depends on the state of the material (i.e., depends on the nodal freedoms \(\ddot{q}\)). Therefore, the equilibrium equations (Eq. (8)) are non-linear.

The displacements (torsion angle) at the two ends of the 1D system (\(n\) nodes) are specified as at node 1, \(\theta_1 = 0\), at node \(n\), \(\theta_n = \Delta\), where \(\Delta\) is the specified loading (torsion angle).

Discrete approximation in time dimension is used to solve Eq. (8). When the state (\(\tilde{q}\)) at time \(t\) is given, the state (\(\tilde{q}_{t+\Delta t}\)) at time \(t + \Delta t\) can be obtained by solving
\[\tilde{K}_{t+\Delta t} \ddot{q}_{t+\Delta t} + \tilde{C}_{t+\Delta t} \frac{(\ddot{q}_{t+\Delta t} - \ddot{q}_t)}{\Delta t} = 0, \quad (9)\]
where \((\ddot{q}_{t+\Delta t} - \ddot{q}_t)/\Delta t\) takes the place of \(\ddot{q}_{t+\Delta t}\) for approximation. Such an approximation (also called backward difference) is unconditionally stable in the implicit numerical calculation.\(^{31}\) Equation (9) can be rearranged into
\[\left(\tilde{K}_{t+\Delta t} + \frac{\tilde{C}_{t+\Delta t}}{\Delta t}\right) \ddot{q}_{t+\Delta t} - \frac{\tilde{C}_{t+\Delta t}}{\Delta t} \ddot{q}_t = 0. \quad (10)\]

Since the element stiffness depends on nodal freedoms, the stiffness \(\tilde{K}\) is not a constant matrix but depends on the magnitudes of the nodal freedoms. Therefore, Eq. (10) is a system of nonlinear equations and needs an iteration scheme to solve. The Newton–Raphson iteration method\(^{12}\) is a common method to solve such nonlinear equations.

The Newton–Raphson iteration method is used to solve a nonlinear equation like
\[\Phi = \varphi - \lambda = 0, \quad (11)\]
where \(\varphi\) is a nonlinear function of the unknown \(q\) while \(\lambda\) is a constant. If an approximation (initial) value of the unknown is given, \(q_{(i)}\), an improved solution, \(q_{(i+1)}\), can be obtained through a Taylor expansion of Eq. (11) for the first order approximation, let
\[\Phi(q_{(i+1)}) = \Phi(q_{(i)}) + \frac{\partial \Phi}{\partial q} q_{(i)} \Delta q_{(i)} = 0\]
\[\implies \Delta q_{(i)} = -\frac{\partial \Phi}{\partial q}^{-1} \Phi(q_{(i)}) \quad (12)\]
\[= -\left(\frac{\partial (\varphi - \lambda)}{\partial q}\right)^{-1} \Phi(q_{(i)}) = -\left(\frac{\partial \varphi}{\partial q}\right)^{-1} \Phi(q_{(i)}) \implies q_{(i+1)} = q_{(i)} + \Delta q_{(i)}.\]

This means that the approximation value in the \((i+1)th\) iteration step, \(q_{(i+1)}\), can be obtained by that in the \(i\)th iteration step, \(q_{(i)}\), through Eq. (12). The iteration process repeats until the following convergent criterion is reached
\[
\{\Phi[q_{(i+1)}]\}^2 < \text{a small value}. \quad (13)
\]
The small circle on the energy curve in Fig. 2 is the spinodal point of the non-convex energy. When a perfect filament is loaded up to this point, the FEM simulation has ill-conditioned stiffness and it is not possible to find the solutions properly through iteration. In our current simulations, several selected elements are treated as defects by reducing their cross section area by a certain percentage so that new phase can be nucleated there.

The capability of the non-local FEM simulation in describing the flagella phase transition is demonstrated. Moreover, the effects of the interface and the viscous relaxation on the phase transition are also discussed.

The simulated torque-twist curve of a filament (length 20 µm) is shown in Fig. 4. After the first elastic deformation of the N phase, there is a load drop in the curve characterizing the nucleation of the SC phase. During the growth of the SC phase, the torque is zero, which means that the two phases are coexisted and on the Maxwell line. When the SC phase grows to occupy the whole filament, the torque experiences a sudden change due to interface annihilation. Further loading leads to elastic deformation of the SC phase.

According to the torque response (Fig. 4), the twist distributions of the phase nucleation and growth are shown in Fig. 5. It is seen that after initial elastic loading (loadings 1-2), an SC phase nucleates from the N phase (loading 3). Then the SC phase grows and coexists with the N phase. The equilibrium twists of these two phases are 0 rad/µm and 4 rad/µm, respectively. There is a transition zone (interface) between the two phases, whose thickness is around 1.2 µm. During the coexistence of the two phases, the SC phase grows via the interface propagation when the torsion loading increases (loadings 3-5 in Fig. 5).

A loading-unloading cycle is shown in Fig. 6. There is a torque jump (phase annihilation, with the arrow up) in the unloading curve while a torque drop (phase nucleation, with the arrow down) appears in the loading curve. It is noted that a loop is formed by the loading and unloading curves. That means some elastic energy is dissipated during the instability processes (phase nucleation and annihilation), which is transferred to heat.

According to the torque response of the unloading, the simulated twist distribution is shown in Fig. 7. With the torsion unloading, the SC phase shrinks via the interface propagation (unloadings 1-3). When the phase shrinks to a critical small size (around two times the interface thickness), the phase is annihilated suddenly (unloading 3-5). The filament returns to the initial state (N phase).
We decrease the gradient energy by decreasing $g$ from 1.2 $\mu$m to 0.08 $\mu$m which is comparable with the experimentally observed interface thickness (0.2 $\mu$m–0.08 $\mu$m). By comparing the simulated twist distributions of Fig. 5 ($g = 1.2$ $\mu$m) and Fig. 8 ($g = 0.08$ $\mu$m), we can see that the interface thickness decreases with decreasing $g$. The decrease in the interface thickness means that the interface occupies less volume and has less interfacial energy. This must affect the processes of phase nucleation and phase annihilation. In other words, the changes in the interface properties (governed by $g$ in the current model) affect the phase transition.

In the above simulation results, the external loading time $t$ is much longer than the material characteristic time (viscosity time scale $t_r$ in Eq. (4)). So, the above simulated twist profiles are the equilibrium configurations at different torsion loadings. However, when a sudden torsion load is applied, the twist distribution would evolve as shown in Fig. 9.

The typical simulated twist profiles in the 330 time steps after the sudden loading are shown in Fig. 9 (time step $\Delta t = 0.5$ s). At initial equilibrium configuration (black line $t = 0$ in Fig. 9), the twists of the coexisting two phases are the equilibrium values: 0 rad/$\mu$m and 4 rad/$\mu$m, respectively, while the total torsion angle of the filament is 24 radian. When the torsion loading is suddenly applied (see solid circle for $t = 1\Delta t$), extra elastic twists happen in both phases (the twists of the two phases increase instantaneously). At this time, the driving force reaches a maximum as shown in Fig. 10. With the increases of time $t$, the SC phase grows via interface propagation and the extra elastic twists of the two phases (see $t = 1\Delta t$–300$\Delta t$ in Fig. 9 decrease); the driving force also decreases with time (Fig. 10). Finally, the filament reaches a new equilibrium configuration (the volumes of the SC and N phases are changed) and the driving force decreases to zero.

In summary, we introduce a non-convex non-local viscoelasticity model and implement it in FEM simulations to describe the flagella phase transition between the N phase and the SC phase. The advantages of the model lie in three aspects: The non-convex elastic energy can describe the material instability involved in the phase transition; non-local gradient energy governs the thickness and the energy of the interface (transition zone) between the two coexisting phases; viscous dissipation is included to consider the relaxation process associated with non-equilibrium conditions, e.g., dynamic phase transition under sudden loading. This model and the FEM code provide a basic tool to investigate the behaviors of flagella under various boundary conditions.

In real experiments, flagella phase transition can be very complicated, e.g. the flagella phase transition is cyclic in a flowing fluid and the deformation includes both twisting and bending. Further studies are still needed to achieve a full understanding of the flagella’s behaviors. The main conclusions of our preliminary results are summarized as follows.

The nonconvex nonlocal elasticity model and the developed FEM code are able to simulate the transformation process of a bio-filament phase nucleation, propagation and annihilation. The simulation captures the main features of the observation of Hotani’s experiment (torque accumulation corresponds to phase nucleation, torque drop corresponds to phase growth, forward and backward transition).

The effect of the interfacial properties (interface thickness and energy) on the phase transition can be properly described by the non-local theory. The interfacial properties affect both the twist profiles and the
torque responses during phase nucleation and phase annihilation.

Non-equilibrium evolution of the two coexisting phases under dynamic loadings can be captured in the non-local FEM simulation based on the viscoelasticity framework.

This work was supported by the Hong Kong University of Science and Technology and the National Natural Science Foundation of China (10902013).