The Correspondence between Ferroelectric Molecular (FLM) Material and the Bio-molecular Worm-Like Chain (WLC) Model for Designing a Novel Switching Device

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Abstract

Taking the advantage of the comparison between the organic worm-like chain (WLC) model and inorganic ferroelectric molecular (FLM) materials, we can explore the similarity between them through the Hamiltonians. The authors suggest that the evolution of molecular domain boundaries and the domain switching of ferroelectric chevron structures are closely related. This will be helpful for developing bimolecular based nano-devices through the analogy to the existing ferroelectric opto-electronic properties.

Keywords: ferroelectric, worm like chain

1. Introduction

In general, the correspondence relation between two systems is very useful for understanding the unknowns for both systems. Since it is in our interest to study the possible bio-nano device as the next generation components, it now becomes a reasonable choice to look for the correspondence between the existing opto-electronic elements to the candidate of the bio-components. Several approaches have been adopted by using the phenomenological WLC model with the appropriate parameters for this purpose [1-3]. However, unlike the well known FLM material, it is usually difficult to derive the complete governing equations for studying the biomolecular dynamics process. In the past few decades, researchers have discussed the basic concepts behind the domain switching phenomena in FLM materials and proposed several models, especially for chevron structures. Further, the switching bistabilities is well explained by c-director switching rather than chevron switching [4-7].

Therefore, it is natural that we start from the comparison of the Hamiltonian functions for both the WLC model and FLM materials. Based on this, it is possible to speculate the transient behavior of the WLC bimolecular string using the stability criteria well defined for FLM materials. The similarity between the Hamiltonians of biomolecular strings and ferroelectric materials can provide a clue to understand the mechanism of the formation of the biomolecular strings from inorganic materials. This will be helpful in the physical interpretation of the molecular dynamics, as well as a key for developing bimolecular based nano-devices through the analogy to the existing ferroelectric opto-electronic properties.

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2. Theory

Following the notation definitions from **[3]** and **[7]**, Figure 1(a) reveals the ferroelectric chevron structure of FLM, and Figure 1(b) shows the configuration of WLC biomolecular string. Here a local order parameter ρ is defined for WLC, and the FLM is characterized by the tilt angle θ. ρ=0 indicates a completely collapsed state, and ρ=1 represents the total extension state.

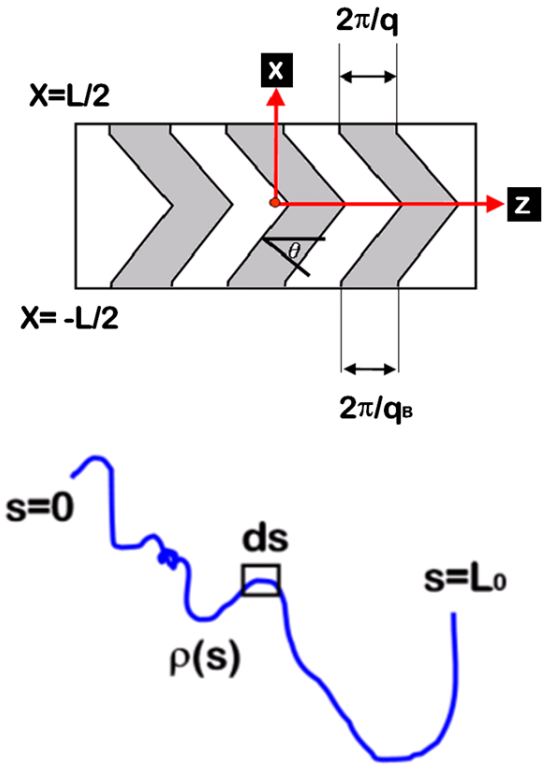

Figure 1: Definition of parameters: (a) ferroelectric chevron structure [7] (b) WLC model [3]

One can write down the Hamiltonian of the FLM materials as **[7]**:

$$\int_{-L/2}^{L/2}\left(\frac{K}{2}(\frac{\partial\theta}{\partial x})^2+Z(\theta;g)\right)dx \qquad (1)$$

where K is the Frank bend elastic constant and Z(θ;g) is a potential function of the tilt angle θ for the chevron structure, and the parameter g originates from the definition of the FLM layer strain. g is the control parameter related with the strain of the FLM structure. On the other hand, the coarse-grained Hamiltonian for WLC can be introduced as **[3]**:

$$\int_0^{L_0}\left(\frac{c}{2}(\frac{\partial\rho}{\partial s})^2+W(\rho;f)\right)ds \qquad (2)$$

where c is a positive constant and W(ρ;f) is the effective double-well potential function with the force f as the control parameter. The reason for considering a double-well potential is that there are two stable states for WLC while ρ=0 or 1. It is obviously that Equations (1) and (2) have the same Hamiltonian form. Moreover, both FLM and WLC show similar "domain-switching" phenomena. Therefore, the state variable θ of FLM materials can be assumed to be analogous to the order parameter ρ (as the state variable) of the WLC model. Now we examine the similarity of the kernels between the mathematical forms of the two potential functions. The potential function W of the WLC model is **[3]**:

$$W(\rho;f)=\frac{\Gamma}{2}\left(\frac{1}{4}\rho^4+\frac{1}{4}(1-2k(f))\rho^2+(\frac{k(f)}{3}-\frac{1}{2})\rho^3\right) \qquad (3)$$

where Γ devotes the material property and k(f)≡tanh(δ)/2. As a comparison, the potential function Z(θ;g) of a FLM material can be written as **[7]**:

$$Z(\theta;g)=\frac{B}{2}\left(\frac{1}{4}\theta^4+\frac{1}{2}(g^2-1)\theta^2+\frac{(1-g^2)^2}{4}\right) \qquad (4)$$

where B is the compressibility of FLM and $g \equiv q/q_B$. Back to the Equation (3), we note that there is a third-older term ρ^3 in W (ρ;f), and it is impossible to eliminate this term since |k(f)|<1/2. On the contrary, there is no restriction to assign $g^2=1$ if one would like to eliminate the constant term for Z (θ;g). However, this will also eliminate the θ^2 term. Therefore, expanding the control term k(f) in Taylor series, the potential function W(ρ;f) now becomes W(ρ;δ) **[8]**:

$$2W(\rho;\delta)\big|_{\delta\to 0}/\Gamma = \left(\frac{1}{4}\rho^4 - \frac{1}{2}\rho^3 + \frac{1}{4}\rho^2 + \delta\rho^2\left(\frac{\rho}{6} - \frac{1}{4}\right)\right) \quad (5)$$

Suffix δ→0 represents the state for control parameter δ approaching to a critical value. Similar treatment with a linear transformation (i.e. η≡1-θ) leads to the FLM potential function with the shifting of the origin (a, b) under small strain approach g→1:

$$2Z(\eta;g)\big|_{g\to 1}/B = \begin{pmatrix} \frac{1}{4}\eta^4 + (a-1)\eta^3 + \frac{3}{2}(a-1)^2\eta^2 + (a-1)^3\eta \\ +\left(\frac{a^4}{4} - a^3 + \frac{3}{2}a^2 - a + b - \frac{1}{4}\right) \end{pmatrix} \quad (6)$$

Now there three parameters (δ, a, b) can control the topological structures of the two functions. Discussions on the effects of these parameters and the correspondence between the two will be revealed in the next sections.

3. Results and Discussions

Figure 2 shows a comparison between the two potential functions for WLC model (blue line, Equation (5) W(ρ;δ)) and FLM material (red line, Equation (6) Z(η;g)) under several typical parameters and the δ→0, g→1 criterions. At the present moment, there are two stable states for the WLC model (ρ=0,1) and one stable state for FLM materials (η=1/2). However, the control parameter δ can transform the W function from two positive definitive stable states into one positive definitive stable state ($dW/d\rho=0$ and $d^2W/d\rho^2>0$). Most important of all, if we release the constrains for g→0, then compare Equation (5) W(ρ;δ) and Equation (4) Z(θ;g), these two functions are both with two stable solutions and share the same topological structures, as function W shown in Figure 2.

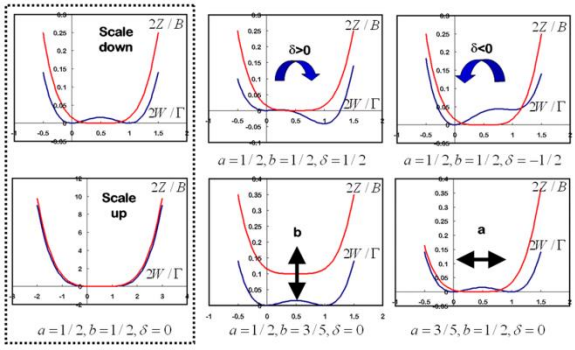

Figure 2: Comparison of potentials between WLC model W and FLM material Z

This is quite naturally since FLM exhibits the bistabilities. The importance of these arguments is through the controlling of the g for FLM material, and the controlling of the δ parameters is the necessary technique to manipulate the molecular nano device, in which one can operate either in two stables modes or in one stable mode. In addition, the capabilities for the controlling the δ parameters in the WLC model can modulate the energy requirements that switching from one mode into another mode. For example, the stretching length of the molecular string (ρ=1) will be preferred for δ>0 and vice versa for (ρ=0) under δ<0.

Based on the correspondence between the WLC model and FLM materials, now we can proceed the analogy between the two systems. Table 1 is the basic corresponding group for WLC and FLM (based on Equations (1) and (2)). Since the modulation of the liquid crystal is the balance between the Frank elasticity constant K and the applied electric field, this corresponding tells us that one should adjust the c parameter (related with the mechanical properties of the molecular structure) of the WLC molecular for the novel nano device. Along with the previous discussion, complete control parameters for WLC and FLM are (c, δ) and (K, g), respectively. The former (c and K) are the internal properties related to the molecular structure, and the later (δ and g) are external control parameters. In the future, techniques on the theory of catastrophe **[9]** can be applied to design the nano device in a more sophisticated way.

Table 1: Basic corresponding between WLC and FLM

Physical terms	WLC	FLM
Bending Properties	c (eq.2)	K (eq.1)
State Variable	ρ (eq.2)	θ (eq.1)
Local coordinate	s (eq.1)	x (eq.1)
Compressible Properties	Γ (eq.3)	B (eq.4)
Operating criterions	δ→0	g→1

Now we can compare the stabilities criteria for the FLM and the WLC. The operating of the nano device must consider the stabilities of the system and find the appropriate way for the controlling of the system. Take FLM as an example, a chevron number is proposed to indicate the chevron structure, and the related optical performance of the FLM device can be written as **[7]**:

$$\Sigma_{\mathrm{FLM}} \equiv \frac{BL^2\varepsilon}{4\pi^2 K} \tag{7}$$

where ε is the strain within the FLM device due to the dislocation shown in Figure 1. Because the Hamiltonian for FLM and WLC share the similar form, the evolution of the domain boundary and the stabilities of the molecular structures can be cross-explained and cross-examined from both sides. Here we need to discuss about the parameter g. The definition of g follows $g \equiv q/q_B$ which originates from the definition of the layer strain. Base on this, strain in the FLM becomes $\varepsilon \sim (1-g^2)/2$, and, therefore, Equation (7) now becomes

$$\Sigma_{\mathrm{FLM}} = \frac{BL^2}{8\pi^2 K}(1+g)(1-g) \tag{8}$$

Equation (8) serves for the criteria on the FLM opto-electronic device. Based on the similarity between $\delta \rightarrow 0 \propto g \rightarrow 1$, we can assign $\delta=m(1-g)$, where m is a proportional constant. According to the corresponding principles, we can have Equation (9) that describes for the bio-molecular devices.

$$\Sigma_{\mathrm{WLC}} = \frac{1}{m^2}\frac{\Gamma L_0^2}{8\pi^2 c}\delta(2m-\delta) \qquad (9)$$

Other correspondence, such as the dynamic motion equation, can be written for WLC from the known FLM motion equation (second order PDE $\partial\theta/\partial t=v^2\partial^2\theta/\partial s^2-\theta(\theta-g/2)(\theta-1)+\xi(s,t)$ **[7]**). By doing this, the domains like structures of WLC indicates in Figure 1 can be explained in more details. Domain boundaries clearly emerge in the WLC model during the releasing and stretching processes of the molecular strings, and this model yields thermodynamically stable globular structure rather relaxes the complete molecular string into the $\rho=1$ state. Through the correspondence, the motion equation for the WLC predicts the existing of the clustering behaviors, in which similar the formation of the domains walls in FLM. Therefore, the motion of boundary walls in the WLC model can be a good model to explain the existence and formation of the crystallized globular structures in molecular strings (typical size of **100 nm** for a long DNA chain), and the novel opto-electric properties can be modulated through these crystallized globular structures. As a final remark, Equation (9), like Equation (8) served for FLM, becomes the key for the operating of biomolecular-based nano devices.

4. Conclusions

The comparison between the WLC model and ferroelectric materials is presented. The correspondence in this paper is used not only to propose complementary equations, but also to study the physical properties of the two systems. We have found an analogy between the WLC model and FLM materials, and the study of the physical properties of FLC might leads to designing bimolecular devices. Based on the similarity between the Hamiltonians of the both, we could explain the evolution of domain boundaries and stabilities of molecular structures in detail and examine using two different approaches. One could control the WLC type bimolecular as a nano device through the similarity to the commercialized optoelectronic ferroelectric materials.

Acknowledgment

This work was sponsored by the Ministry of Science and Technology of the Republic of China, under grand NSC99-2221-E-164-007, NSC100-2221-E-164 -002 and MOST 103-2221-E-164 -002.

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