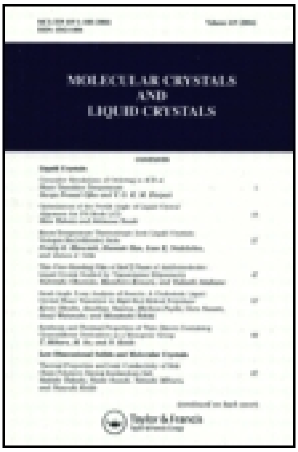

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Effects of Weak Anchoring on the Elastic Distortion of a Biaxial Nematic Liquid Crystal on Surface Grooves

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A generalized form of anisotropic surface energy for the description of biaxial nematic liquid crystals is proposed, and the effects of weak anchoring on the elastic distortion of the biaxial nematic material on surface grooves is investigated as an extension of our previous work on the effects of strong anchoring [Zhang Z. D., & Ye W. J. (2009). Liq. Cryst.*,* 36*, 885–888]. With some approximations for the elastic constants, we obtain a more general expression for the additional elastic distortion energy per unit area induced by the minor director $\vec{m}$. The results show that finite polar anchoring can provide an important contribution to the additional elastic distortion energy, and the additional term reduces to our previous result with strong polar anchoring.*

Keywords Biaxial nematic liquid crystal; elastic distortion; surface groove; weak anchoring

Introduction

As early as in 1972, Berreman [1] studied the contribution of elastic origin to the surface anchoring of a nematic liquid crystal (LC) in the presence of a non-flat surface. He assumed that the nematic director on the unidirectionally grooved substrate is oriented along the grooves, minimizing the bulk elastic energy. In his analysis, he assumed that in a first approximation the surface can be described by a sinusoidal wave of wave number $q = 2\pi/\lambda$ and amplitude A, where λ is the spatial periodicity of the surface. The surface azimuthal anchoring energy, obtained by assuming that $Aq \ll 1$ and $K_1 = K_2 = K_3 = K$(the elastic constants), is proportional to $\sin^2\phi$ (ϕ being the angle between the director at infinity and direction of surface grooves), and it varies strongly with the amplitude A and the wave number q. Since Berreman's theory is the first theoretical study on surface anchoring attributed to non-flat surface geometry and his model is simple enough, it has served as a starting point for subsequent numerous theories [2–11] as well as experimental

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studies [12–14] in this field. In particular, Fukuda et al. [8] re-examined the theoretical treatment of Berreman's theory for the surface anchoring induced by grooves with infinite polar anchoring (strong anchoring) and argued that Berreman's assumption of negligibly small azimuthal distortion of nematic is not valid. He showed that the Berreman's model considering azimuthal distortion yields a surface anchoring energy proportional to $\sin^4 \phi$ and implies that surface grooves alone cannot contribute to the surface-anchoring coefficient in the usual Rapini–Papoular sense. Furthermore, he considered the contribution from surface-like elasticity characterized by K_{24} and showed that the surface-like elastic term is a nonzero contribution to the Rapini–Papoular anchoring energy [9,10]. In addition, Faetti [2] and our group [11] investigated the effects of finite polar anchoring at a grooved interface on the azimuthal anchoring energy in the frame of Berreman's original theory and Fukuda et al.'s theory respectively. Both studies showed that the finite polar anchoring could lead to an important contribution to the azimuthal anchoring energy.

Biaxial nematic LCs are a fascinating condensed matter phase that have baffled scientists engaged in the challenge of demonstrating its actual existence for more than 30 years, and which have only recently been found experimentally [15–17]. The preferred direction of the orientation of molecules in the biaxial phase is described by an orthonormal triad of director vector fields $\vec{n}$, $\vec{m}$, and $\vec{l}$ [18]. On one hand, surface anchoring of an LC has been among the most important subjects of both uniaxial and biaxial nematic research [15–17,19–21] and elastic distortions of the LC adjacent to non-flat surfaces have long been argued as the most important source of surface anchoring. On the other hand, by extending Fukuda et al.'s [8] method to the biaxial nematic LCs, we found that when the main director $\vec{n}$ is anchored along a surface groove, an additional distortion energy is induced by the minor director $\vec{m}$ [22].

In this paper, extending our preliminary work [22], we investigate the effects of finite polar anchoring on surface azimuthal anchoring energy of biaxial nematic LCs.

Theoretical Basis

The finite anchoring energy per unit area, which accounts for the interaction of a uniaxial nematic LC with the substrate, is defined as [11,23]

$$f_{su} = w_p(\vec{n} \cdot \vec{\nu})^2, \tag{1}$$

where $\vec{n}$ is the director at the surface and $\vec{\nu}$ denotes the local unit vector perpendicular to the surface. Now we are going to obtain a generalized formula suitable to biaxial nematics by means of a tensor phenomenological description of surface anchoring of LCs.

In a proper chosen coordinate system denoted by the unit vectors $\vec{e}_i'$, $i = 1, 2, 3$, the tensor order parameter $\overleftrightarrow{Q}$ is diagonal with elements

$$\bar{Q}_{11} = -\frac{1}{3}(S - T), \quad \bar{Q}_{22} = -\frac{1}{3}(S + T), \quad \bar{Q}_{33} = \frac{2}{3}S,$$

and

$$\bar{Q}_{ij} = 0 \quad \text{if } i \neq j.$$

Biaxial nematics are described by the two order parameters S and T, whereas uniaxial nematics are described by only one order parameter S,in which case the uniaxial axis is chosen along $\vec{e}'_3$. Consequently, the general expression for the tensor order parameter $\overleftrightarrow{Q}$ of a biaxial nematic can be written as [24]

$$\overleftrightarrow{Q} = S\left(\vec{n}\otimes\vec{n} - \frac{1}{3}\overleftrightarrow{I}\right) + \frac{1}{3}T\left(\vec{l}\otimes\vec{l} - \vec{m}\otimes\vec{m}\right) \tag{2}$$

where $\overleftrightarrow{I}$ is the unit tensor.

In the treatment of grooved surface for uniaxial nematics [11,23], finite polar anchoring was assumed to be completely isotropic in the local tangent plane of the grooved surface. Following this point of view, the most general quadratic form describing isotropic substrates is [25,26]

$$f_{sb} = c_1\vec{\nu}\cdot\overleftrightarrow{Q}\cdot\vec{\nu} + c_2 tr\,Q^2 + c_3(\vec{\nu}\cdot\overleftrightarrow{Q}\cdot\vec{\nu})^2 + c_4\vec{\nu}\cdot\overleftrightarrow{Q}^2\cdot\vec{\nu}, \tag{3}$$

where c_i $(i = 1,\ 2,\ 3,\ 4)$ are constants. By substituting Eq. (2) into Eq. (3), the finite anchoring energy per unit area for the interaction of a biaxial nematic LC with the substrate takes the form

$$f_{sb} = w_p(\vec{n}\cdot\vec{\nu})^2 + w_b(\vec{m}\cdot\vec{\nu})^2 + w'_b(\vec{l}\cdot\vec{\nu})^2, \tag{4}$$

where terms that do not depend on director vector fields $\vec{n}$, $\vec{m}$, or $\vec{l}$ have been neglected. In Eq. (4), w_p,w_b, and w'_b depend on the order parameters S and T, but they are treated as constants in our approaches of this paper, based upon the continuum theory of biaxial nematics [27,28].

We consider a surface groove whose shape can be described by

$$x = \zeta(y, z) = A\sin[q(y\cos\phi + z\sin\phi)] \tag{5}$$

where A and q have been defined above, and ϕ describes the angle between the groove direction and the z-axis (see Fig. 1). We assume $Aq \ll 1$ and a biaxial nematic is filled in the semi-infinite region, $x > \zeta(y,z)$. The components of the local unit vector normal to the surface are given by

$$\begin{aligned}\nu_x &\approx 1,\\ \nu_y &\approx -Aq\cos\phi\cos[q(y\cos\phi + z\sin\phi)],\\ \nu_z &\approx -Aq\sin\phi\cos[q(y\cos\phi + z\sin\phi)].\end{aligned} \tag{6}$$

Let the orientation of the director triad at the uniform state be

$$\vec{l} = (1, 0, 0);\quad \vec{m} = (0, 1, 0);\quad \vec{n} = (0, 0, 1). \tag{7}$$

When the distortion of biaxial nematics from the uniform state is small enough, we can write down the director triad as

$$\vec{l} = (1, l_y, l_z);\quad \vec{m} = (m_x, 1, m_z);\quad \vec{n} = (n_x, n_y, 1). \tag{8}$$

As $\vec{l}$, $\vec{m}$, and $\vec{n}$ are orthonormal, one has

$$m_x = -l_y;\quad n_y = -m_z;\quad l_z = -n_x. \tag{9}$$

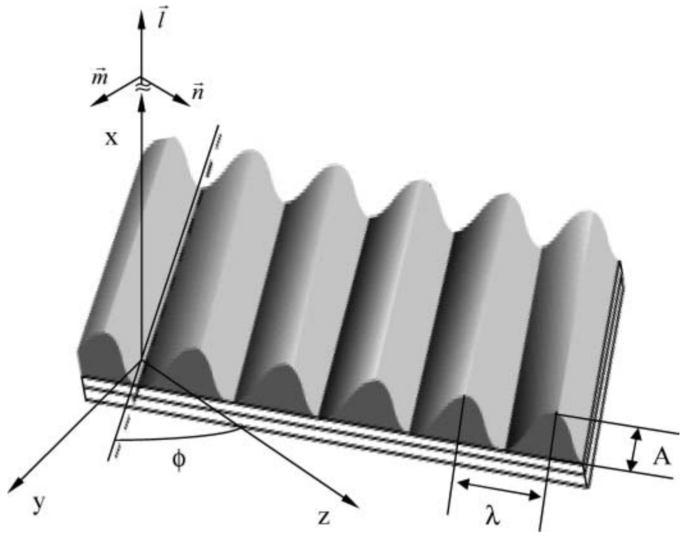

Figure 1. Schematic representation for a sinusoidally shaped groove surface with amplitude A and spatial periodicity λ. At infinite $x \to \infty$, there are $\vec{l} = (1, 0, 0)$, $\vec{m} = (0, 1, 0)$, and $\vec{n} = (0, 0, 1)$. Φ is the angle between z-axis and the direction of the grooves, i.e., the angle made between the main director $\vec{n}$ at infinity and the direction of surface grooves.

Thus, only three out of the six perturbations in Eq. (8) are independent. By substituting Eqs. (6), (8), and (9) into Eq. (4), one has

$$\begin{aligned} f_{sb} &= w_p \{n_x - Aq \sin\phi \cos[q(y\cos\phi + z\sin\phi)]\}^2 \\ &\quad + w_b\{l_y + Aq\cos\phi\cos[q(y\cos\phi + z\sin\phi)]\}^2, \end{aligned} \tag{10}$$

where w_b' term, which does not depend on the director triad (on condition that $Aq \ll 1$), has been neglected.

According to Saupe [27], the elasticity of biaxial nematics is described by 15 elastic constants, among which there are 12 constants corresponding to director distortions in the bulk and three constants amount to surface-like elasticity. The elastic-free energy density, as given in Ref. [27], is

$$\begin{aligned} g_b = \sum_{a,b,c} \frac{1}{2}[K_{aa}(\vec{a}\cdot\nabla\vec{b}\cdot\vec{c})^2 + K_{ab}(\vec{a}\cdot\nabla\vec{a}\cdot\vec{b})^2 + K_{ac}(\vec{a}\cdot\nabla\vec{a}\cdot\vec{c})^2] \\ + C_{ab}(\vec{a}\cdot\nabla\vec{a})\cdot(\vec{b}\cdot\nabla\vec{b}) + k_{0,a}\nabla\cdot(\vec{a}\cdot\nabla\vec{a} - \vec{a}\nabla\cdot\vec{a}), \end{aligned} \tag{11}$$

where the summation is over a cyclic permutation of three directors and indices. Hereafter, the director fields are denoted by $\vec{l}$, $\vec{m}$, and $\vec{n}$ for convenience. Choosing n_x, n_y, and l_y as the three perturbations, the elastic-free energy density is written as [22,28]

$$\begin{aligned} g_b = \frac{1}{2}K_{LL}(n_{y,x})^2 + \frac{1}{2}K_{MM}(n_{x,y})^2 + \frac{1}{2}K_{NN}(l_{y,z})^2 + \frac{1}{2}K_{LM}(l_{y,x})^2 + \frac{1}{2}K_{MN}(n_{y,y})^2 \\ + \frac{1}{2}K_{NL}(n_{x,z})^2 + \frac{1}{2}K_{ML}(l_{y,y})^2 + \frac{1}{2}K_{NM}(n_{y,z})^2 + \frac{1}{2}K_{LN}(n_{x,x})^2 + C_{LM}n_{x,x}n_{y,y} \end{aligned}$$

$$- C_{MN} l_{y,y} n_{x,z} + C_{NL} n_{y,z} l_{y,x} - 2k_{0,L}(l_{y,z} n_{x,y} - l_{y,y} n_{x,z})$$
$$+ 2k_{0,M}(l_{y,z} n_{y,x} - l_{y,x} n_{y,z}) + 2k_{0,N}(n_{x,y} n_{y,x} - n_{x,x} n_{y,y}) \,, \tag{12}$$

where the indices L, M, and N are used instead of a, b, and c.

Using the full variational principle for the total free energy, we can derive the equilibrium conditions:

$$K_{MM} n_{x,yy} + K_{NL} n_{x,zz} + K_{LN} n_{x,xx} + C_{LM} n_{y,xy} - C_{MN} l_{y,yz} = 0, \tag{13a}$$
$$K_{LL} n_{y,xx} + K_{MN} n_{y,yy} + K_{NM} n_{y,zz} + C_{LM} n_{x,xy} + C_{NL} l_{y,xz} = 0, \tag{13b}$$
$$K_{NN} l_{y,zz} + K_{LM} l_{y,xx} + K_{ML} l_{y,yy} - C_{MN} n_{x,yz} + C_{NL} n_{y,xz} = 0, \tag{13c}$$

together with the condition at the surface ($x \sim 0$):

$$\frac{\partial g_b}{\partial n_{x,x}} \delta n_x + \frac{\partial g_b}{\partial n_{y,x}} \delta n_y + \frac{\partial g_b}{\partial l_{y,x}} \delta l_y = \frac{\partial f_{sb}}{\partial n_x} \delta n_x + \frac{\partial f_{sb}}{\partial l_y} \delta l_y. \tag{14}$$

Eq. (14) leads to explicit boundary conditions at $x \sim 0$, i.e.,

$$K_{LL} n_{y,x} + 2k_{0,M} l_{y,z} + 2k_{0,N} n_{x,y} = 0, \tag{15a}$$
$$K_{LN} n_{x,x} + C_{LM} n_{y,y} - 2k_{0,N} n_{y,y} = \frac{\partial f_{sb}}{\partial n_x}, \tag{15b}$$
$$K_{LM} l_{y,x} + C_{NL} n_{y,z} - 2k_{0,M} n_{y,z} = \frac{\partial f_{sb}}{\partial l_y}. \tag{15c}$$

Saupe [27] and Singh et al. [29] pointed that in the uniaxial phase, there are

$$K_{LN} = K_{MN} = K_1, \tag{16a}$$
$$K_{MM} = K_{LL} = K_2, \tag{16b}$$
$$K_{NL} = K_{NM} = K_3, \tag{16c}$$
$$C_{LM} = K_1 - K_2, \tag{16d}$$
$$C_{MN} = C_{NL} = 0, \tag{16e}$$
$$2k_{0,N} = K_{24} - K_2, \tag{16f}$$

and

$$K_{NN} = K_{LM} = K_{ML} = 0. \tag{17}$$

Taking Eq. (16) into account, Eqs. (13a) and (13b) lead to

$$K_1 n_{x,xx} + K_2 n_{x,yy} + K_3 n_{x,zz} + (K_1 - K_2) n_{y,xy} = 0, \tag{18a}$$
$$K_2 n_{y,xx} + K_1 n_{y,yy} + K_3 n_{y,zz} + (K_1 - K_2) n_{x,xy} = 0. \tag{18b}$$

Eqs. (18a) and (18b) completely correspond to Eqs. (7) and (8) in our previous work for the uniaxial nematics [11]. (In order to use Eq. (12), we assume that $\vec{n} = (n_x,\ n_y,\ 1)$ instead of $\vec{n} = (1,\ n_y,\ n_z)$ as in [11].)

Singh et al. [29] predicted that on a molecular theory, the seven elastic constants, namely, K_{LN}, K_{MN}, K_{MM}, K_{LL}, K_{NL}, K_{NM}, and C_{LM} are of the order of the values found in the uniaxial nematic phase, and among the three C constants associated with mixed models of deformation, C_{MN} and C_{NL} are about one order of magnitude smaller than C_{LM}. Thus, in the present work on biaxial nematics, we assume that Eqs. (18a) and (18b) can still be used approximately, and $C_{MN} = C_{NL} = 0$, i.e., the mixed elastic constants can be neglected except C_{LM}. This approximation means that the differences of splay elastic constant and twist one are neglected for both $\vec{l}$ and $\vec{m}$ directors. Consequently, Eq. (13c) becomes

$$K_{LM} l_{y,xx} + K_{ML} l_{y,yy} + K_{NN} l_{y,zz} = 0. \tag{19}$$

Now the coupling between n_i ($i = x, y$) and l_y is neglected for the equations in bulk. To the same order of approximation, we neglect the influence of surface-like elasticity $k_{0,M}$ in the boundary conditions (15a) and (15c). Thus, explicit boundary conditions, at $x \sim 0$, are given by Eqs. (20) and (21), that is,

$$K_{24} n_{x,y} - K_2(n_{x,y} - n_{y,x}) = 0, \tag{20a}$$

$$K_1(n_{x,x} + n_{y,y}) - K_{24} n_{y,y} = 2w_p \{n_x - Aq \sin\phi \cos[q(y\cos\phi + z\sin\phi)]\}, \tag{20b}$$

and

$$K_{LM} l_{y,x} = 2w_b \{l_y + Aq \cos\phi \cos[q(y\cos\phi + z\sin\phi)]\}. \tag{21}$$

Note that Eqs. (20a) and (20b) completely correspond to Eqs. (9) and (10) in [11]. As a result, the effects of finite polar anchoring on the azimuthal anchoring energy appear partly in a way of the uniaxial nematics by solving Eqs. (18a) and (18b) under the boundary conditions: Eqs. (20a) and (20b) at the surface $x \sim 0$ and the ultimate conditions $n_x = n_y = 0$ at $x \to \infty$ (see Fig. 1). Once that surface-like elasticity $k_{0,L}$ is also neglected, the azimuthal anchoring energy for biaxial nematics can be written as

$$f(\phi) = f_a(\phi) + \Delta f(\phi), \tag{22}$$

where $f_a(\phi)$ is given by Eq. (20) in [11], representing azimuthal anchoring energy of the uniaxial nematics; $\Delta f(\phi)$ is the distortion energy of the minor director $\vec{m}$ when the main director $\vec{n}$ is anchored along surface grooves.

Results and Discussion

In order to obtain the additional azimuthal anchoring energy $\Delta f(\phi)$ induced by the elastic distortion of the minor director, one can obtain the analytical solution of Eq. (19) with the boundary conditions given by Eq. (21) at $x \sim 0$, and $l_y = 0$ at $x \to \infty$,

$$l_y = -Aq \cos\phi R \cos[q(y\cos\phi + z\sin\phi)] \exp[-qxh(\phi)], \tag{23}$$

with $h(\phi) = \sqrt{(K_{ML}\cos^2\phi + K_{NN}\sin^2\phi)/K_{LM}}$, and

$$R = \frac{2w_b}{qK_{LM}h(\phi) + 2w_b}. \tag{24}$$

From Eq. (12), an additional distortion energy per unit area $\Delta f(\phi)$ is written as

$$\Delta f(\phi) = \frac{1}{4} A^2 q^3 \cos^2\phi K_{LM} h(\phi) R^2. \tag{25}$$

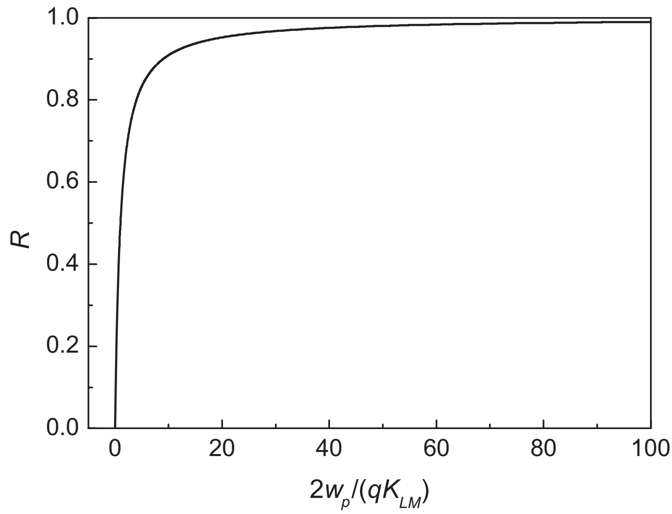

Figure 2. The dependence of R on the values of $2w_b/(qK_{LM})$.

Obviously, with strong polar anchoring, i.e., $w_b \to \infty$, $R = 1$, Eq. (25) reduces to

$$\Delta f(\phi) = \frac{1}{4} A^2 q^3 \cos^2 \phi K_{LM} h(\phi), \tag{26}$$

which is the result given by Eq. (23) in [22].

In one-constant model for the minor director, one has [22,27]

$$K_{NN} = K_{ML} = K_{LM}. \tag{27}$$

In this case, $h(\phi) = 1$, and Eq. (25) reduces to

$$\Delta f(\phi) = \frac{1}{4} A^2 q^3 \cos^2 \phi K_{LM} R^2, \tag{28}$$

with

$$R = \frac{2w_b}{qK_{LM} + 2w_b} \tag{29}$$

Equation (29) shows that$R$depends only on $2w_b/(qK_{LM})$, and the dependence of R on the values of $2w_b/(qK_{LM})$ is given in Fig. 2. It is clear that R increases with the value of $2w_b/(qK_{LM})$. In addition, from Eq. (28), we can conclude that the azimuthal anchoring energy $\Delta f(\phi)$ increases as the value of $2w_b/(qK_{LM})$ increases.

Further assuming that $\phi = 0$, Eq. (28) reduces to

$$\Delta f(\phi = 0) = \frac{1}{4} A^2 q^3 K_{LM} R^2, \tag{30}$$

with $R = \frac{2w_b}{qK_{LM}+2w_b}$. In the case of strong polar anchoring, i.e., $w_b \to \infty$, Eq. (30) reduces to $\Delta f(\phi = 0) = \frac{1}{4} A^2 q^3 K_{LM}$, which is the result given by Eq. (24) in [22].

Equation (30) holds that in anchoring the $\vec{n}$ director along the grooves, the $\vec{m}$ director is distorted, and the distortion energy is approximately given by Eq. (30). In uniaxial nematic

LCs, this distortion energy is zero, i.e., the state of a uniaxial nematic characterized by the director $\vec{n}$ is uniform in space. In the biaxial nematic LCs, Eq. (30) gives a distortion energy that must be overcome in anchoring the $\vec{n}$ director along the grooves.

Conclusion and Discussion

In this work, extending our previous work [22], we have investigated the elastic distortion of the biaxial nematic LCs on surface grooves with finite polar anchoring and considered the effect of polar anchoring on the additional elastic distortion energy induced by the minor director $\vec{m}$. We showed that the finite polar anchoring could provide an important contribution to the additional elastic distortion energy (Eq. (25) and Fig. 2). Moreover, considering the infinite anchoring strength, the results are consistent with those in [22].

We note that homeotropic alignment is another important anchoring condition. In order to realize homeotropic alignment to biaxial nematic LCs, different methods developed successfully for the uniaxial nematic phase have been used widely. One example is of a special polymer being coated on the substrate [19,21,30–32]. A process of weak rubbing may be used to produce surface grooves, which provide a preferred direction, so that a monodomain state with a uniformly tilted director field can be built up above the bend Fréedericksz transition in a material with negative dielectric anisotropy. But we have known, for the uniaxial nematic phase, homeotropic alignment on the surface is not destroyed by the surface grooves in Berreman's approximation [33]; i.e., Eq. (22) gives

$$f_a(\phi) = \frac{1}{4}A^2q^3\sqrt{K_1K_3}. \tag{31}$$

Thus, the disturbance of the minor director $\vec{m}$ induced by the surface grooves is direct, and homeotropic anchoring is more difficult than homogeneous anchoring for the biaxial nematic LCs.

On the other hand, the three constants, K_{LM}, K_{ML}, and K_{NN} are much smaller than the value of the constants found in the uniaxial nematic phase [29] and $|R| < 1$, therefore $\Delta f(\phi)$ is a perturbation term in Eq. (22). Thus, we understand in a sense, why homogenous alignment for biaxial nematics has been obtained in a wide range of choices [19,21,30–32].

Acknowledgments

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