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The elastic distortion and stability of biaxial nematic liquid crystal on the surface grooves

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Fukuda *et al.* reexamined the Berreman's model which attributes the surface anchoring to the elastic distortion of the uniaxial nematic liquid crystal induced by the grooves of a surface. They showed that at the variance with the assumption made in the original approach of Berreman, the azimuthal distortion of the director cannot be considered as negligibly small. Now this method is generalized to the biaxial nematic liquid crystals, with some approximations for the elastic constants. We obtain an additional term in the elastic distortion energy per unit area which depends on the second power of the cosine of the angle made between the main director **n** at infinity and the direction of the surface grooves. This additional term describes the distortion energy of the minor director **m** induced by the surface grooves when the **n** director is anchored exactly along the grooves. We have studied the stability of the **n** director around the grooves, and in one-constant model for each director the stability condition is that the elastic constant of the **n** director is the maximum.

Keywords: Berreman's model; biaxial nematic liquid crystal; groove; elastic distortion

As early as 1972, Berreman (*1*) presented the first theoretical study on surface anchoring attributed to non-flat surface geometry and resultant elastic distortion of a uniaxial nematic liquid crystal. In his analysis he considered a rubbed surface, and assumed that, in a first approximation, it can be approximated by a sinusoidal wave of wave vector $q = 2\pi/\lambda$ and amplitude A, where λ is the spatial periodicity of the surface. With the assumption that $K_1 = K_3 = K$ and that $qA<<1$, he showed that the surface topography is responsible for an equivalent anchoring energy

$$w_B = \frac{1}{2}K(qA)^2 q, \tag{1}$$

characterized by an easy direction parallel to the grooves. Numerous studies have been carried out to understand the effect of the surface topography on the molecular orientation of liquid crystalline phases (*2–4*). Recently, the experimental realization of a sub-micrometre-scale surface grooved with sufficient geometrical precision has again provoked interest in the notion of surface anchoring attributable to the geometry of the surface (*5–8*). In particular, Fukuda *et al.* (*5*) showed that Berreman's model should yield a surface energy proportional to the fourth power of the sine of the angle made between the director at infinity and the direction of the surface grooves.

Biaxial nematic liquid crystals are a fascinating condensed matter phase that has baffled scientists engaged in the challenge of demonstrating its actual existence for more than 30 years, and which has only recently been found experimentally (*9–11*). In this preliminary work, we apply the method proposed by Fukuda *et al.* (*5*) to the biaxial nematic liquid crystals, with some approximations for the elastic constants.

The elasticity of biaxial nematics is described by 15 elastic constants: 12 of these correspond to director distortions in the bulk and three constants amount to surface-like elasticity (*12–14*). The elastic free energy density, as given in (*12*), is

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

where the summation is over a cyclic permutation of the three directors and indices. Hereafter, the director fields are denoted by **l**, **m** and **n** for convenience. Let the orientation of the director triad at the uniform state be

$$\mathbf{l} = (1,0,0); \quad \mathbf{m} = (0,10); \quad \mathbf{n} = (0,0,1). \tag{3}$$

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

$$\mathbf{l} = (1,l_y,l_z); \quad \mathbf{m} = (m_x,1,m_z); \quad \mathbf{n} = (n_x,n_y,1). \tag{4}$$

As **l**, **m**, **n** are orthonormal, one has

$$m_x = -l_y; \quad n_y = -m_z; \quad l_z = -n_x. \tag{5}$$

Thus, only three out of the six perturbations in Equation (4) are independent. Following Singh *et al.* (*15*), the elastic free energy density is written as

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$$
\begin{aligned}
g_b =& \frac{1}{2}K_{LL}(m_{z,x})^2 + \frac{1}{2}K_{MM}(n_{x,y})^2 + \frac{1}{2}K_{NN}(l_{y,z})^2 \\
&+ \frac{1}{2}K_{LM}(l_{y,x})^2 + \frac{1}{2}K_{MN}(m_{z,y})^2 + \frac{1}{2}K_{NL}(n_{x,z})^2 \\
&+ \frac{1}{2}K_{ML}(l_{y,y})^2 + \frac{1}{2}K_{NM}(m_{z,z})^2 + \frac{1}{2}K_{LN}(n_{x,x})^2 \\
&- C_{LM}n_{x,x}m_{z,y} - C_{MN}l_{y,y}n_{x,z} - C_{NL}m_{z,z}l_{y,x} \\
&- 2k_{0,a}(l_{y,z}n_{x,y} - l_{y,y}n_{x,z}) - 2k_{0,b}(l_{y,z}m_{z,x} - l_{y,x}m_{z,z}) \\
&- 2k_{0,c}(n_{x,y}m_{z,x} - n_{x,x}m_{z,y}) \qquad (6)
\end{aligned}
$$

where the indices L, M and N are used instead of a, b and c. In fact, Equation (6) can be obtained directly from Equation (2) with conditions given by Equations (4) and (5). The equations of equilibrium are

$$-K_{LL}m_{z,xx} - K_{MN}m_{z,yy} - K_{NM}m_{z,zz} + C_{LM}n_{x,xy} + C_{NL}l_{y,xz} = 0, \qquad (7a)$$

$$-K_{MM}n_{x,yy} - K_{NL}n_{x,zz} - K_{LN}n_{x,xx} + C_{LM}m_{z,xy} + C_{MN}l_{y,yz} = 0, \qquad (7b)$$

$$-K_{NN}l_{y,zz} - K_{LM}l_{y,xx} - K_{ML}l_{y,yy} + C_{MN}n_{x,yz} + C_{NL}m_{z,xz} = 0. \qquad (7c)$$

Saupe (*12*) and Singh *et al.* (*15*) pointed that in the uniaxial phase, there are

$$K_{LN} = K_{MN} = K_1, \qquad (8a)$$

$$K_{MM} = K_{LL} = K_2, \qquad (8b)$$

$$K_{NL} = K_{NM} = K_3, \qquad (8c)$$

$$C_{LM} = K_1 - K_2, \qquad (8d)$$

$$C_{MN} = C_{NL} = 0 \qquad (8e)$$

$$2k_{0,c} = K_{24} - K_2, \qquad (8f)$$

and

$$K_{NN} = K_{LM} = K_{ML} = 0. \qquad (9)$$

Similar approximations can also be found in (*16*). Taking Equations (5) and (8) into account, Equations (7b) and (7a) lead to

$$K_1n_{x,xx} + K_2n_{x,yy} + K_3n_{x,zz} + (K_1 - K_2)n_{y,xy} = 0, \qquad (10a)$$

$$K_2n_{y,xx} + K_1n_{y,yy} + K_3n_{y,zz} + (K_1 - K_2)n_{x,xy} = 0. \qquad (10b)$$

Equations (10a) and (10b) correspond completely to Equations (7) and (8) in (*5*). (In order to use Equation (6), we assume that $\mathbf{n} = (n_x, n_y, 1)$ instead of $\mathbf{n} = (1, n_y, n_z)$ as in (*5*).)

In this preliminary work for the biaxial nematics, we assume that Equations (10a) and (10b) 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 the **l** director and the **m** director. Consequently, Equation (7c) becomes

$$K_{LM}l_{y,xx} + K_{ML}l_{y,yy} + K_{NN}l_{y,zz} = 0. \qquad (11)$$

In accordance with $\mathbf{n} = (n_x, n_y, 1)$, we should consider a surface groove whose shape can be described by

$$x = \zeta(y, z) = A\sin[q(y\cos\phi + z\sin\phi)], \qquad (12)$$

where ϕ is the angle between z-axis and the direction of the grooves (see Figure 1). A biaxial nematics is filled in the infinite region $x>\zeta(y, z)$. We further assume that the **l** director at the surface is perpendicular to it, so that one has

$$l_y = -Aq\cos\phi\cos[q(y\cos\phi + z\sin\phi)], \qquad (13a)$$

$$l_z = -Aq\sin\phi\cos[q(y\cos\phi + z\sin\phi)]. \qquad (13b)$$

According to Equations (5) and (13b), the boundary condition of n_x at the surface is given by

$$n_x = Aq\sin\phi\cos[q(y\cos\phi + z\sin\phi)]. \qquad (14)$$

There should be an additional boundary condition at the surface $x \sim 0$ (see (*5*, *17*)),

$$\frac{\partial g_b}{\partial n_{x,x}}\delta n_x + \frac{\partial g_b}{\partial n_{y,x}}\delta n_y + \frac{\partial g_b}{\partial l_{y,x}}\delta l_y = 0. \qquad (15)$$

As n_x and l_y is fixed at the surface and no condition is imposed on δn_y, Equation (15) gives

$$\frac{\partial g_b}{\partial n_{y,x}} = 0, \qquad (16)$$

so that one has

$$K_{LL}n_{y,x} + 2k_{0,b}l_{y,z} + 2k_{0,c}n_{x,y} = 0. \qquad (17)$$

Equations (10a), (10b) and (11) are derived by setting $C_{MN} = C_{NL} = 0$ in Equations (7a)–(7c), so that the coupling between n_i (i = x, y) and l_y is neglected. To the same order of approximation, we neglect the influence of surface-like elasticity $k_{0,b}$. Thus, Equations (10a) and (10b) can be solved by the boundary condition at the surface, obtaining (by Equations (8f) and (17)),

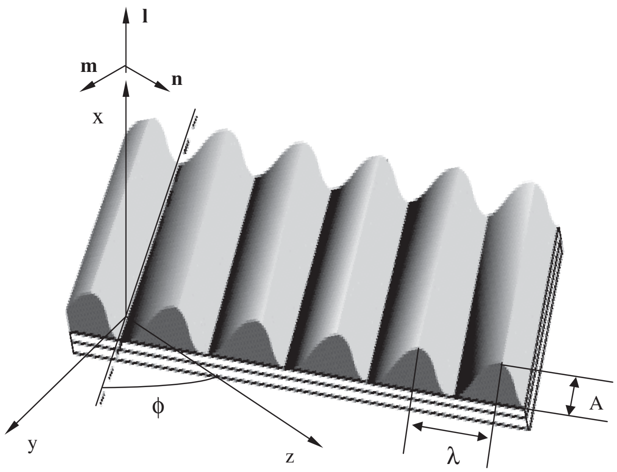

Figure 1. Schematic representation for a sinusoidally shaped groove surface with the amplitude A and the spatial periodicity λ. At infinite $x \to \infty$, there are $\mathbf{l} = (1,0,0)$, $\mathbf{m} = (0,1,0)$ and $\mathbf{n} = (0,0,1)$. Here, ϕ is the angle between the z-axis and the direction of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

$$K_{24} n_{x,y} + K_2(n_{y,x} - n_{x,y}) = 0 \quad (18)$$

and the boundary condition $n_x = n_y = 0$ at $x \to \infty$(see Figure 1). The solution can be found in (*17*). For simplicity, we write only the solution on condition that $K_{24} = 0$,

$$n_x = Aq \sin\phi e^{-qxg_1(\phi)} \cos[q(y\cos\phi + z\sin\phi)], \quad (19)$$

$$n_y = \frac{Aq\sin\phi\cos\phi}{g_1(\phi)} e^{-qxg_1(\phi)} \sin[q(y\cos\phi + z\sin\phi)], \quad (20)$$

with $g_1(\phi) = \sqrt{\cos^2\phi + (K_3/K_1)\sin^2\phi}$, and anchoring energy per unit area reads

$$f(\phi) = \frac{1}{4} K_3 A^2 q^3 \frac{\sin^4\phi}{g_1(\phi)}. \quad (21)$$

Now, one can find the analytical solution of Equation (11) with the boundary conditions given by Equation (13a) at $x \sim 0$, and $l_y = 0$ at $x \to \infty$,

$$l_y = -Aq\cos\phi\cos[q(y\cos\phi + z\sin\phi)]\exp[-qxh(\phi)], \quad (22)$$

with $h(\phi) = \sqrt{(K_{ML}\cos^2\phi + K_{NN}\sin^2\phi)/K_{LM}}$. From Equation (6), an additional distortion energy per unit area is written as

$$f_b(\phi) = \frac{1}{4} A^2 q^3 \cos^2\phi K_{LM} h(\phi). \quad (23)$$

In fact, this additional term is not influenced by setting $K_{24} = 0$. When $\phi = 0$, Equation (23) reduces to

$$f_b(\phi = 0) = \frac{1}{4} A^2 q^3 K_{ML}. \quad (24)$$

In the biaxial nematic phase, fast switching between different birefringent states may be possible because birefringence can be changed by the rotation of the minor director **m** while the main director **n** is fixed (*18, 19*). In anchoring the **n** director along the grooves, the **m** director is distorted and the distortion energy is approximately given by Equation (24). In the uniaxial nematic liquid crystals, this distortion energy is zero, that is, the state of uniaxial nematics characterized by the director **n** is uniform in space. In the biaxial nematic liquid crystals, Equation (24) gives a distortion energy which must be overcome in anchoring the **n** director along the grooves.

Now we study stability conditions for aligning the biaxial nematics on the grooves. For simplicity, the direction of the grooves is assumed to be parallel to the z-axis of a Cartesian reference frame. The elastic free energy density is approximated by neglecting the mixed elastic constants and surface-like elasticity; in one-constant model for each director (*12, 20*),

$$K_{LL} = K_{MN} = K_{NM}, \quad (25a)$$

$$K_{MM} = K_{NL} = K_{LN}, \quad (25b)$$

$$K_{NN} = K_{LM} = K_{ML}. \quad (25c)$$

Some discussions for one-constant model of the biaxial nematics can be found in (*21*). Now, the director **n** is disturbed by a small angle $\delta\alpha$ in the direction of the grooves, that is,

$$\mathbf{n} = (-\sin(\delta\alpha)\sin\theta, \sin(\delta\alpha)\cos\theta, \cos(\delta\alpha)), \quad (26)$$

where θ depends on x and y. The **m** director is assumed to be described by

$$\mathbf{m} = (\cos\theta, \sin\theta, 0), \quad (27)$$

and the **l** director is determined by $\mathbf{l} = \mathbf{m} \times \mathbf{n}$. Through a long analytical deduction, we arrive at the following expression for the free energy density,

$$g_b = \frac{1}{2} K_{NN}\left[(\theta_{,x})^2 + (\theta_{,y})^2\right] + \frac{1}{2}(K_{LL} - K_{NN})\sin^2(\delta\alpha)\left[(\theta_{,x})^2 + (\theta_{,y})^2\right], \quad (28)$$

where a term of the fourth order of $\sin(\delta\alpha)$ has been dropped. When α = 0, with the assumption that the **m** director at the sinusoidally grooved surface is always tangential to the surface, the Berreman's model gives

Equation (24) directly, replacing K_{LM} by K_{NN}. Under disturbance of $\delta\alpha$, one stability condition is

$$\frac{d^2 g_b}{d(\delta\alpha)^2}|_{\delta\alpha=0}>0,$$

and one has $K_{LL}>K_{NN}$. If we still use Equation (23) to represent the director **n**, but the director **l** is given by

$$\mathbf{l} = (\cos\theta, \sin\theta, 0), \tag{29}$$

we obtain the other stability condition $K_{MM} > K_{NN}$.

In fact, in one-constant model for each director of the biaxial nematics, three elastic constants are

$$K_n = \frac{1}{2}(K_{LL} + K_{MM} - K_{NN}), \tag{30a}$$

$$K_l = \frac{1}{2}(K_{NN} + K_{MM} - K_{LL}), \tag{30b}$$

$$K_m = \frac{1}{2}(K_{NN} + K_{LL} - K_{MM}). \tag{30c}$$

Thus, the stability condition of the **n** director around the grooves is the elastic constant of the **n** director is the maximum.

In summary, a method that treats the elastic distortion of the uniaxial nematic liquid crystal induced by the grooves of a surface has been generalized to the biaxial nematic liquid crystals, with some approximations for the elastic constants. We have obtained an additional term in the elastic distortion energy per unit area which depends on the second power of the cosine of the angle made between the main director at infinity and the direction of the surface grooves. This additional term describes the distortion energy of the minor director induced by the surface grooves when the main director is anchored exactly along the grooves. Finally, we have studied the stability of the main director around the grooves, and in a one-constant model for each director the stability condition is the elastic constant of the main director that is the maximum.

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