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Influence of Surface Geometry of Grating Substrate on Director in Nematic Liquid Crystal Cell*

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Abstract *The director in nematic liquid crystal cell with a weak anchoring grating substrate and a strong anchoring planar substrate is relative to the coordinates x and z. The influence of the surface geometry of the grating substrate in the cell on the director profile is numerically simulated using the two-dimensional finite-difference iterative method under the condition of one elastic constant approximation and zero driven voltage. The deepness of groove and the cell gap affect the distribution of director. For the relatively shallow groove and the relatively thick cell gap, the director is only dependent on the coordinate z. For the relatively deep groove and the relatively thin cell gap, the director must be dependent on the two coordinates x and z because of the increased elastic strain energy induced by the grating surface.*

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Key words: grating substrate, director, elastic constant, two-dimensional finite-difference iterative method

Display characteristics of a liquid crystal displays (LCDs) are mainly decided by the director profile of liquid crystal (LC) in this cell. Surface anchoring plays an essential role in the director's distribution.[1−2] The rubbing technique is a common method to align the LC molecules on the surface of substrate in the manufacture of LCDs.[3] However, to achieve some desirable anchoring properties, the surface of substrate is treated as a grating surface. Theoretical and experimental studies on the grating surface are always important subjects.[4−13]

In 1972, Berreman[14] studied the interaction between a nematic liquid crystal (NLC) and a grating surface using the continuum theory. The shape of the cross section perpendicular to the groove direction is taken as a sinusoidal curve. Based on the simple model of a grating surface proposed by Berreman, some investigators reexamined the theory and analyzed the distribution of director.[15−17] In our previous works,[18−19] we considered that the shape of cross section is taken as cosinusoidal curve

$$z = \delta \cos(qx)\,, \tag{1}$$

where x is the direction perpendicular to the groove of the grating substrate, $q = 2\pi/\lambda$ is the wave vector of the surface structure, λ is the pitch of grating surface, and δ is its amplitude. The anchoring properties of grating substrate can be expressed by the equivalent anchoring energy formula per unit area of the projected plane of the grating surface

$$g_s = \frac{1}{2}W_1(\boldsymbol{n}\cdot\boldsymbol{j})^2 + \frac{1}{2}W_2(\boldsymbol{n}\cdot\boldsymbol{i})^2\,, \tag{2}$$

where $\boldsymbol{i}$, $\boldsymbol{j}$ are the basic vectors along ox, oy axis, respectively, $W_1 = A_1 - 4\pi^3\bar{k}\delta^2/\lambda^3$ and $W_2 = A_2$ are the equivalent anchoring strength coefficients, A_1 and A_2 are anchoring strengths of the grating substrate and $\bar{k}$ is the geometric mean value of the splay elastic constant k_{11} and the twist elastic constant k_{22}, i.e. $\bar{k} = \sqrt{k_{11}\cdot k_{22}}$. In the following theoretical analysis, this formula is used to calculate the anchoring energy of the grating substrate.

Our selected LC cell structure and the Cartesian coordinate system are shown in Fig. 1. A NLC is confined between a weak anchoring grating substrate and a strong anchoring planar substrate. The original point of Cartesian coordinate system is laid in the center of the projected plane of grating substrate. The LC molecules orient along the normal direction of the grating surface and the anchoring energies corresponding to different directions are A_1 and A_2, respectively. The LC molecules on the planar substrate are homogeneous alignment. The deforma-

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tion of director in the LC layer without an applied electric field can be described as $\boldsymbol{n} = (\cos\theta\cos\phi, \cos\theta\sin\phi, \sin\theta)$. Here, θ and ϕ are the tilt and the twist angle of director, respectively, and they are dependent on x and z, rewritten as $\theta = \theta(x, z)$, $\phi = \phi(x, z)$.

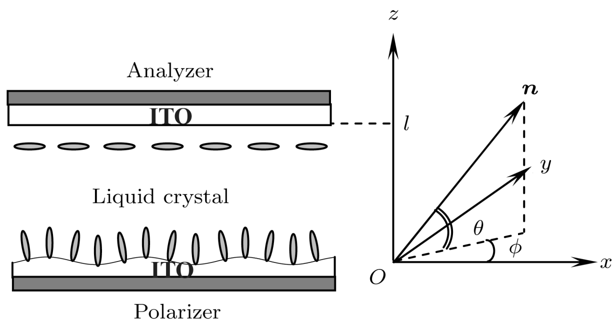

Fig. 1 Structure of liquid ccrystal cell and coordinate system.

The Gibbs free energy of the NLC cell consists of two parts: elastic free energy and surface free energy. The elastic free energy is

$$G_{\text{elastic}} = \int_V g_{\text{elastic}} \mathrm{d}V = \int_{-L_y}^{L_y} \mathrm{d}y \int_{-L_x}^{L_x} \mathrm{d}x \int_{\delta\cos(qx)}^{l} g_{\text{elastic}} \mathrm{d}z\,, \tag{3}$$

where L_x and L_y are two half widths of the grating substrate, g_{elastic} is the density of the elastic free energy in per unit bulk and can be expressed as

$$g_{\text{elastic}} = \frac{1}{2}k_{11}(\vec{\nabla}\cdot\vec{n})^2 + \frac{1}{2}k_{22}(\vec{n}\cdot\vec{\nabla}\times\vec{n})^2 + \frac{1}{2}k_{33}(\vec{n}\times\vec{\nabla}\times\vec{n})^2\,, \tag{4}$$

where k_{11}, k_{22}, and k_{33} denote splay, twist, and bend elastic constants respectively. Introducing some new signs $S_\theta = \sin\theta$, $C_\theta = \cos\theta$, $S_\phi = \sin\phi$, $C_\phi = \cos\phi$, $\theta'_x = \partial\theta/\partial x$, $\theta'_z = \partial\theta/\partial z$, $\phi'_x = \partial\phi/\partial x$, $\phi'_z = \partial\phi/\partial z$, we can simplify the expression of the density of the elastic free energy as

$$\begin{aligned} g_{\text{elastic}} = {} & \frac{1}{2}k_{11}\big\{(S_\theta C_\phi\theta'_x - C_\theta\theta'_z)^2 + C_\theta^2 S_\phi^2 \phi'^2_x + 2C_\theta S_\phi\phi'_x(S_\theta C_\phi\theta'_x - C_\theta\theta'_z)\big\} \\ & + \frac{1}{2}k_{22}\big\{S_\phi^2\theta'^2_x + C_\theta^2(S_\theta C_\phi\phi'_x - C_\theta\phi'_z)^2 - 2C_\theta S_\phi\theta'_x(S_\theta C_\phi\phi'_x - C_\theta\phi'_z)\big\} \\ & + \frac{1}{2}k_{33}\big\{(C_\theta C_\phi\theta'_x + S_\theta\theta'_z)^2 + C_\theta^2(C_\theta C_\phi\phi'_x + S_\theta\phi'_z)^2\big\}\,. \end{aligned} \tag{5}$$

Because the integral interval in Eq. (3) along the oz axis is $[\delta\cos(qx),\, l]$, this will bring some troubles in the theoretical calculation. To overcome this problem, a variable transformation $(x, y, z) \to (x', y', z')$ is introduced as the following

$$x' = x\,, \quad y' = y\,, \quad z' = \frac{z - \delta\cos(qx)}{l - \delta\cos(qx)}l\,. \tag{6}$$

Substituting Eq. (6) into Eq. (3), one can write the following expression of the elastic free energy in the new variable

$$G_{\text{elastic}} = \int_{-L_y}^{L_y} \mathrm{d}y \int_{-L_x}^{L_x} \mathrm{d}x' \int_0^l \tilde{g}_{\text{elastic}} \cdot D\,\mathrm{d}z'\,, \tag{7}$$

where $\tilde{g}_{\text{elastic}}$ is the density of the elastic free energy in the new variable, D is a required factor for transforming the integral variable and can be written by

$$D = \begin{vmatrix} \dfrac{\partial x}{\partial x'} & \dfrac{\partial x}{\partial y'} & \dfrac{\partial x}{\partial z'} \\ \dfrac{\partial y}{\partial x'} & \dfrac{\partial y}{\partial y'} & \dfrac{\partial y}{\partial z'} \\ \dfrac{\partial z}{\partial x'} & \dfrac{\partial z}{\partial y'} & \dfrac{\partial z}{\partial z'} \end{vmatrix} = 1 - \frac{1}{l}\delta\cos(qx')\,. \tag{8}$$

To simply analysis, one elastic constant approximation ($k_{11} = k_{22} = k_{33} = k$) is assumed. In this case, Eq. (5) can be re-expressed as

$$g_{\text{elastic}} = \frac{k}{2}[\theta'^2_x + \theta'^2_z + C_\theta^2(\phi'^2_x + \phi'^2_z) + 2C_\theta^2 S_\phi(\theta'_x\phi'_z - \theta'_z\phi'_x)]\,. \tag{9}$$

The expression of $\tilde{g}_{\text{elastic}}$ is given by

$$\begin{aligned} \tilde{g}_{\text{elastic}} = \frac{k}{2}\big\{ & (\theta'_{x'} + B\theta'_{z'})^2 + E^2\theta'^2_{z'} \\ & + C_\theta^2[(\phi'_{x'} + B\phi'_{z'})^2 + E^2\phi'^2_{z'}] \\ & + 2C_\theta^2 S_\phi E(\theta'_{x'}\phi'_{z'} - \theta'_{z'}\phi'_{x'})\big\}\,, \end{aligned} \tag{10}$$

where

$$E = \frac{l}{l - \delta\cos(qx')} = \frac{1}{D}\,, \quad B = \frac{(l - z')\delta q\sin(qx')}{l - \delta\cos(qx')}\,.$$

Supposing that $g_V = \tilde{g}_{\text{elastic}} \cdot D$ is the bulk density, and considering the surface free energy, we can obtain the whole Gibbs free energy of this system

$$G = \int_{-L_y}^{L_y} \mathrm{d}y \int_{-L_x}^{L_x} \mathrm{d}x' \int_0^l \mathrm{d}z' g_V + \int_{-L_y}^{L_y} \mathrm{d}y \int_{-L_x}^{L_x} \mathrm{d}x' g_s\,, \tag{11}$$

where the expressions of g_V and g_s are

$$\begin{aligned} g_V = \frac{k}{2}\Big\{ & \frac{1}{E}(\theta'_{x'} + B\theta'_{z'})^2 + E\theta'^2_{z'} \\ & + C_\theta^2\Big[\frac{1}{E}(\phi'_{x'} + B\phi'_{z'})^2 + E\phi'^2_{z'}\Big] \\ & + 2C_\theta^2 S_\phi(\theta'_{x'}\phi'_{z'} - \theta'_{z'}\phi'_{x'})\Big\}\,, \end{aligned} \tag{12}$$

$$g_s = \frac{1}{2}W_1\cos^2\theta\sin^2\phi + \frac{1}{2}W_2\cos^2\theta\cos^2\phi\,, \tag{13}$$

where θ and ϕ are the function of x' and z'.

Substituting g_V and g_s into the Euler–Lagrange equations[21]

$$\frac{\partial g_V}{\partial \theta} - \frac{\partial}{\partial x'}\frac{\partial g_V}{\partial \theta'_{x'}} - \frac{\partial}{\partial z'}\frac{\partial g_V}{\partial \theta'_{z'}} = 0\,, \tag{14}$$

$$\frac{\partial g_V}{\partial \phi} - \frac{\partial}{\partial x'}\frac{\partial g_V}{\partial \phi'_{x'}} - \frac{\partial}{\partial z'}\frac{\partial g_V}{\partial' \phi_{z'}} = 0\,, \tag{15}$$

we can obtain the bulk equations respect to θ and ϕ

$$S_\theta C_\theta\Big[(\hat{A}\phi)^2 + \Big[\Big(E\frac{\partial}{\partial z'}\Big)\phi\Big]^2\Big] + \hat{A}^2\theta + \Big(E\frac{\partial}{\partial z'}\Big)^2\theta = 0\,, \tag{16}$$

$$\hat{A}(C_\theta^2\hat{A}\phi) + \Big(E\frac{\partial}{\partial z'}\Big)\Big[C_\theta^2\Big(E\frac{\partial}{\partial z'}\Big)\phi\Big] = 0\,, \tag{17}$$

where

$$\hat{A} = \frac{\partial}{\partial x'} + B\frac{\partial}{\partial z'}\,.$$

At the upper boundary $z' = l$, $\theta(x', l) = 0$, $\phi(x', l) = 0$. θ and ϕ satisfy the following equations at the bottom boundary $z' = 0$,

$$\frac{\partial g_V}{\partial' \theta_{z'}}\Big|_{z'=0} = \frac{\partial g_s}{\partial \theta}\Big|_{z'=0}\,, \tag{18}$$

$$\frac{\partial g_V}{\partial \phi'_{z'}}\Big|_{z'=0} = \frac{\partial g_s}{\partial \phi}\Big|_{z'=0}\,. \tag{19}$$

Substituting Eqs. (12) and (13) into Eqs. (18) and (19), respectively, we have

$$k\Big[\frac{B}{E}\hat{A}\theta + E\theta'_{z'} - C_\theta^2 S_\phi \phi'_{x'}\Big]\Big|_{z'=0} = -[S_\theta C_\theta(W_1 S_\phi^2 + W_2 C_\phi^2)]|_{z'=0}\,, \tag{20}$$

$$k\Big[\frac{B}{E}\hat{A}\phi + E\phi'_{z'} + S_\phi \theta'_{x'}\Big]\Big|_{z'=0} = [S_\phi C_\phi(W_1 - W_2)]|_{z'=0}\,. \tag{21}$$

Based on the above bulk and the boundary equations, the LC director's profile in the NLC cell with a grating substrate and a planar substrate can be calculated. We discuss the deformation of director for the cell with different grating conditions. The elastic constant of LC is $k = 10$ pN. Some parameters of the cell are $l = 5\ \mu$m or $10\ \mu$m, $\lambda = 1\ \mu$m, $\delta = 100$ nm or $1\ \mu$m, $A_1 = 1.0 \times 10^{-4}$ J/m^2, $A_2 = 7.0 \times 10^{-5}$ J/m^2.[17–18] In calculation, we only consider one period along the x direction. According to the different cell gaps and amplitudes, we can obtain four combinations such as $l = 5\ \mu$m and $\delta = 100$ nm, $l = 10\ \mu$m, and $\delta = 100$ nm, $l = 5\ \mu$m, and $\delta = 1\ \mu$m, $l = 10\ \mu$m, and $\delta = 1\ \mu$m. The LC director's distribution are shown in Figs. 2–5.

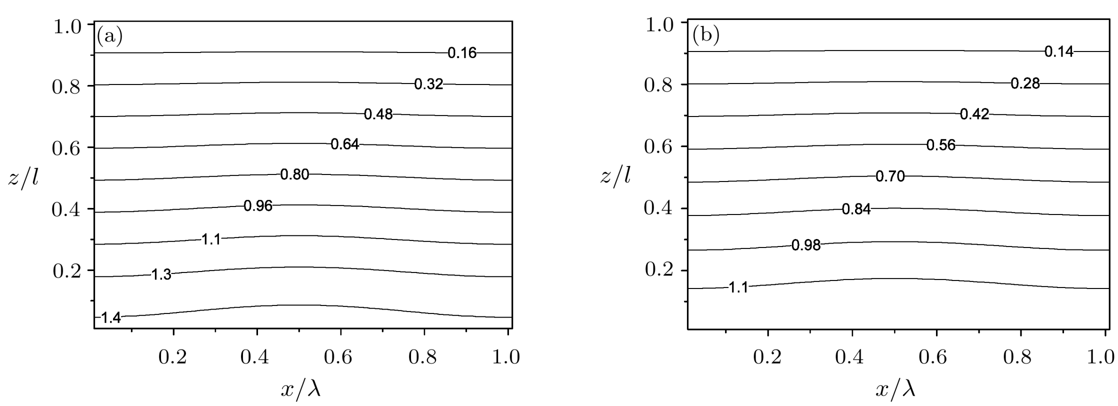

Fig. 2 Distributions of liquid crystal director for $l = 5\ \mu$m and $\delta = 100$ nm. (a) Tilt angle; (b) Twist angle.

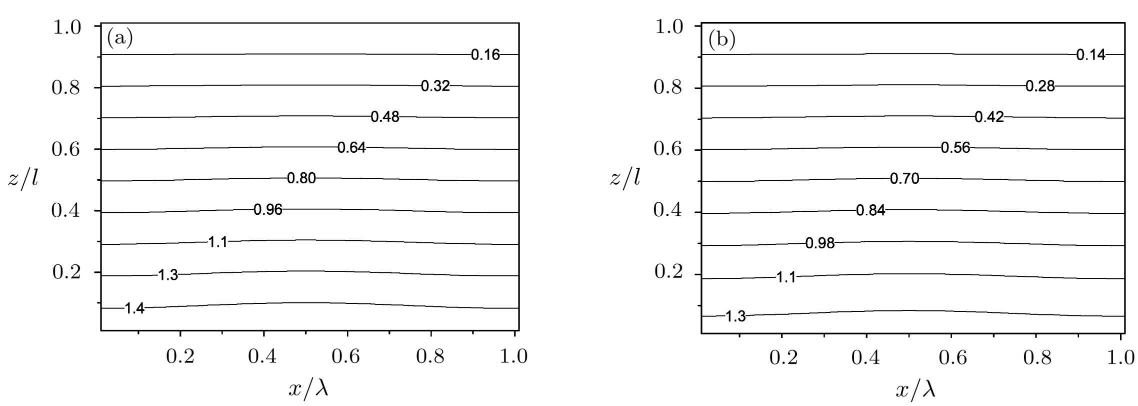

Fig. 3 Distributions of liquid crystal director for $l = 10\ \mu$m and $\delta = 100$ nm. (a) Tilt angle; (b) Twist angle.

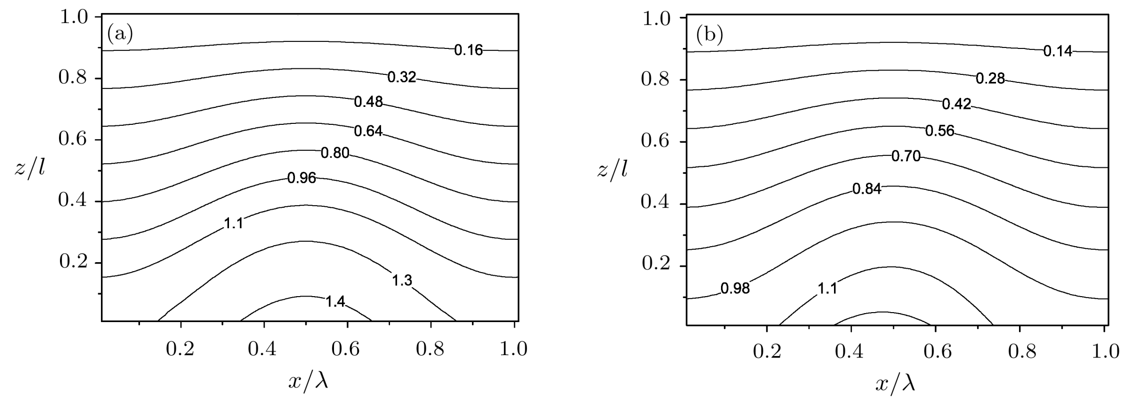

Fig. 4 Distributions of liquid crystal director for $l = 5$ μm and $\delta = 100$ nm. (a) Tilt angle; (b) Twist angle.

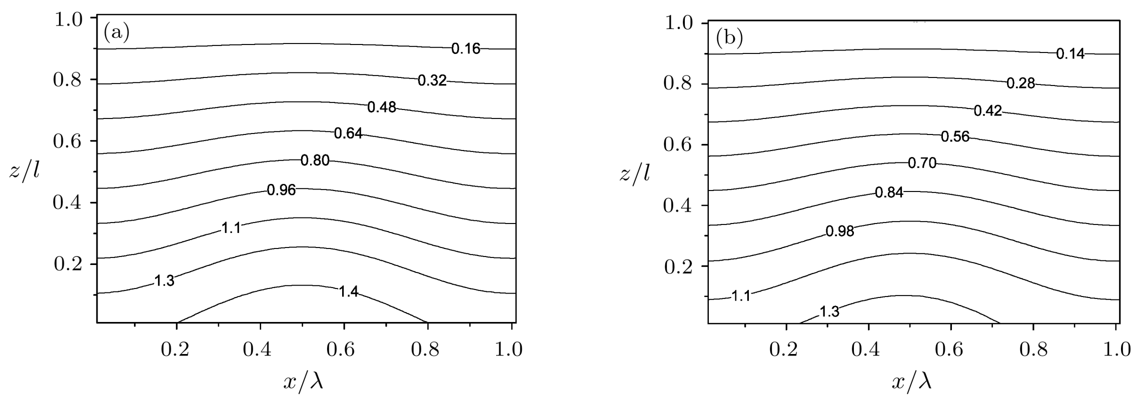

Fig. 5 Distributions of liquid crystal director for $l = 10$ μm and $\delta = 100$ nm. (a) Tilt angle; (b) Twist angle.

The anchoring of the grating substrate is decided by two factors: the interaction potential[22−23] between LC molecules and the molecules of substrate, the increased elastic strain energy[14] induced by grating substrate. The interaction potential leads to the LC molecules along the normal direction of grating surface. The increased elastic strain energy can bring a deviation from the normal direction in the tilt and twist angles.[24] Because the increased elastic strain energy is dependent on the surface geometry of the grating substrate, the different grating surfaces will have the different influences on LC alignment on the grating substrate. These influences can extend to the whole LC layer because of the elasticity of LC. From these figures, we can see this kind of variation. In the cell with the relatively small amplitude and the relatively thick cell gap, the distributions of the tilt angle and the twist angle are linear in the LC layer except a very thin layer near the grating surface from Fig. 3. This means that the tilt angle and the twist angle of director are independent on the coordinate x when the cell has the relative thick LC layer and the relative small amplitude. However, an opposite result is shown in the cell with the thin LC layer and large amplitude. The nonlinear distributions of the tilt angle and the twist angle in the whole LC layer are shown in Figs. 4 and 5. This implies that the tilt angle and the twist angle vary with the coordinates x and z.

In this paper, we give the detailed theoretical analysis on the problem of the grating surface and numerically calculate the distribution of LC director in the NLC cell with a grating substrate and a planar substrate by the two-dimensional finite-difference iterative method. For the relatively shallow groove and the relatively thick cell gap, the director is only dependent on the coordinate z. As a result, some investigations on the NLC cell with grating substrate in this case can be simplified.[12,25] On the contrary, for the case of the relatively deep groove and the relatively thin cell gap, the director must be dependent on the coordinates x and z.

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