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Anchoring properties of substrate with a grating surface*

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The anchoring properties of substrate with a grating surface are investigated analytically. The alignment of nematic liquid crystal (NLC) in a grating surface originates from two mechanisms, thus the anchoring energy consists of two parts. One originates from the interaction potential between NLC molecules and the molecules on the substrate surface, and the other stems from the increased elastic strain energy. Based on the two mechanisms, the expression of anchoring energy per unit area of a projected plane of this grating surface is deduced and called the equivalent anchoring energy formula. Both the strength and the easy direction of equivalent anchoring energy are a function of the geometrical parameters (amplitude and pitch) of a grating surface. By using this formula, the grating surface can be replaced by its projected plane and its anchoring properties can be described by the equivalent anchoring energy formula.

Keywords: anchoring properties, anchoring energy, elastic strain energy, equivalent anchoring energy formula

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1. Introduction

It is well known that liquid crystal cell is fabricated by two pre-treated substrates, between which liquid crystal is filled. Thus, the interaction between liquid crystal molecules and the molecules on the substrate surface is inevitable. In general, this kind of interaction can be described by anchoring energy including the strength and the easy direction of anchoring, which can be seen as the anisotropic part of the interfacial energy.[1] Rapini and Papoular (RP)[2] first put forward the expression of anchoring energy for a one-dimensional case, expressed as $g_s = 1/2A\sin^2\alpha$, where α is the angle between the director on the surface $\boldsymbol{n}$ and easy direction $\boldsymbol{e}$, and A is the anchoring strength. They regarded the substrate surface as a flat plane and assumed that the variation of director on substrate surface occurred in the same flat plane perpendicular to the substrate. As a generalization, there are two modes for the two-dimensional case (such as a twisted NLC cell). One is the single-parameter formula,[3] expressed as

$$g_s = -1/2A(\boldsymbol{n}\cdot\boldsymbol{e})^2, \tag{1}$$

the other is the two-parameter formula,[4,5] given by

$$g_s = 1/2A_\theta\sin^2(\theta^0-\theta_0) + 1/2A_\phi\sin^2(\phi^0-\phi_0), \tag{2}$$

where A_θ and A_ϕ are the tilt anchoring strength and the azimuthal anchoring strength respectively .

For a grating surface, Zhao *et al*[6,7] treated it as a flat plane and gave the corresponding anchoring energy formula through a second-order spherical-harmonic expansion, expressed as

$$g_s = W_\xi(\boldsymbol{n}\cdot\boldsymbol{\xi})^2 + W_\eta(\boldsymbol{n}\cdot\boldsymbol{\eta})^2, \tag{3}$$

where the unit vectors $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$ are in the stationary directions of the second-order anchoring energy. Based on this formula, Guan *et al*[8] studied the threshold and saturation properties of the magnetic-field-induced twist cells. This formula is not related to the geometrical parameters of this grating surface. However, we think that the alignment of nematic liquid crystal (NLC) originates from two mechanisms. One is the interaction potential between NLC molecules and the molecules on the substrate surface,[9] and the other is the elastic strain energy in the bulk of NLC that would be increased if NLC molecules were aligned but not parallel to the groove (or channel) direction.[10,11] Therefore, the anchoring energy consists of two parts.

As far as the first mechanism is concerned, the integration of the ordinary anchoring energy density over the whole grating surface is total anchoring energy and it can be re-expressed as an integration over a

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projected plane of the grating surface, i.e. a flat planar integration. Then we obtain the expression of anchoring energy per unit area of projected plane. This is an anchoring energy density also, but the physical meaning is different from the original one, denoted by $g_s^{(1)}$. For the second mechanism, according to Refs.[11,12], the increased elastic strain energy (per unit area of the projected plane) can be obtained, denoted by $g_s^{(2)}$. Then the total anchoring energy density is

$$g_s = g_s^{(1)} + g_s^{(2)}, \tag{4}$$

where both $g_s^{(1)}$ and $g_s^{(2)}$ are a function of geometrical parameters δ and λ of the grating surface. g_s is referred to as the equivalent anchoring energy density. An NLC cell with a grating surface can be seen as an NLC cell with a flat plane surface by using this formula of g_s. Subsequently, the dependences of the strength and the direction of anchoring on geometrical parameters δ and λ of the grating surface are calculated by computer simulation.

2. Equivalent anchoring energy formula

In this section, we study the anchoring energy corresponding to a grating surface. The geometrical configuration of the substrate with a grating surface is shown in Fig.1.

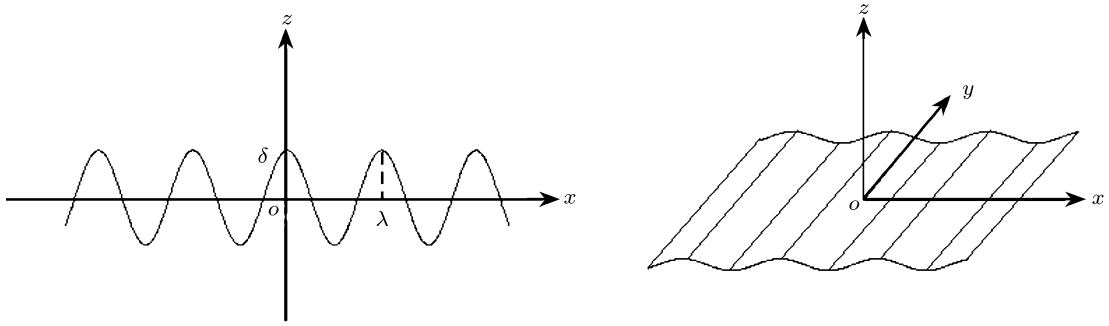


Fig.1. The geometrical configuration of the substrate with a grating surface. (a) The intersectant line between the grating surface and the o-xz plane, δ is the amplitude, λ is the pitch; (b) the whole configuration of the substrate with a grating surface.

The grating long narrow channels are parallel to the oy-axis, and the intersectant line between the grating surface and the x-z plane is a periodic curve. The equation of the grating surface can be written as

$$z = f(x), \tag{5}$$

where $f(x)$ is a periodic function and can be expressed as $f(x) = \sum_{n=1}^{\infty} \delta_n \cos\left(\frac{2n\pi}{\lambda}x\right)$. If all $\delta_2, \delta_3, \cdots$ are very small compared with δ_1, it can be simplified into

$$f(x) = \delta \cos\left(\frac{2\pi}{\lambda}x\right). \tag{6}$$

It is cosinoidal surface (or sinoidal surface), as mentioned in Ref.[10], where δ is the amplitude that is the depth of channel, λ is the pitch that is the distance of two adjacent channels. So the geometry of the grating surface can be described by two parameters δ and λ.

To begin with, we consider the first mechanism. According to Ref.[9], anchoring energy can be seen as the sum of the interaction potentials between surface molecules and liquid crystal molecules, and is related to the equivalent orientation $\boldsymbol{e}$ of surface molecules on the substrate surface. Assuming that the grating surface area element is dS and the unit vector normal to dS is $\boldsymbol{v}$, there are two possibilities for homeotropic anchoring:

i) $\boldsymbol{e}$ is along $\boldsymbol{v}$ and the interaction potential is negative. In this case, the anchoring energy of dS is

$$-\frac{1}{2}A(\boldsymbol{n}\cdot\boldsymbol{v})^2 \mathrm{d}S. \tag{7}$$

ii) $\boldsymbol{e}$ is along the direction of the oy-axis, i.e. parallel to the groove (or channel), and the interaction potential is positive. In this case, the anchoring energy of dS is

$$\left\{\frac{1}{2}A_1(\boldsymbol{n}\cdot j)^2 + \frac{1}{2}A_2(\boldsymbol{n}\cdot\mathbf{j}\times\boldsymbol{v})^2\right\}\mathrm{d}S, \tag{8}$$

where $\boldsymbol{i}$, $\boldsymbol{j}$ and $\boldsymbol{k}$ are the basic vectors along the ox-, oy- and oz-axes respectively, A, A_1, A_2 are the parameters of anchoring strength and greater than zero. We discuss these two cases separately.

i) From Eq.(7), we obtain

$$G_s^{(1)} = \iint\limits_S \left\{ -\frac{A}{2}(\boldsymbol{n}\cdot\boldsymbol{v})^2 \right\} \mathrm{d}S, \tag{9}$$

where S is the area of the grating surface. The expression of $\boldsymbol{v}$ can be obtained by Eq.(5)

$$\boldsymbol{v} = \frac{1}{\sqrt{1+[f'(x)]^2}}(-f'(x)\boldsymbol{i}+\boldsymbol{k}), \tag{10}$$

where $f'(x) = \dfrac{\mathrm{d}f(x)}{\mathrm{d}x}$ and for cosinoidal surface (6) $f' = -2\pi\dfrac{\delta}{\lambda}\sin\left(\dfrac{2\pi}{\lambda}x\right)$. Because the director of liquid crystal can be considered as $\boldsymbol{n} = n_1\boldsymbol{i} + n_2\boldsymbol{j} + n_3\boldsymbol{k}$ in the three-dimensional space, Eq.(9) can be rewritten as

$$G_s^{(1)} = -\frac{A}{2}\iint\limits_S \frac{1}{1+[f'(x)]^2}\left\{-n_1 f'(x)+n_3\right\}^2 \mathrm{d}S. \tag{11}$$

Considering $n_3^2 = 1-n_1^2-n_2^2$ and $v_3\mathrm{d}S = \mathrm{d}x\mathrm{d}y$, where $v_3 = \dfrac{1}{\sqrt{1+[f'(x)]^2}}$, Eq.(11) becomes

$$G_s^{(1)} = \frac{A}{2}\iint\limits_S \left\{ n_2^2\frac{1}{\sqrt{1+[f'(x)]^2}} + n_1^2\frac{1-[f'(x)]^2}{\sqrt{1+[f'(x)]^2}} + 2n_1n_3\frac{f'(x)}{\sqrt{1+[f'(x)]^2}} - \frac{1}{\sqrt{1+[f'(x)]^2}} \right\} \mathrm{d}x\mathrm{d}y, \tag{12}$$

where $S_0 = (2L_x)\times(2L_y)$ denotes the area of the projected plane of the grating surface on the x-y plane, $2L_x$ is the length along the ox-axis, $2L_y$ is the length along the oy-axis.

If the variation of $\boldsymbol{n}$ is very small in the region $|\Delta z \le \delta|$ Eq.(12) can be approximated as

$$\begin{aligned} G_s^{(1)} = {} & \frac{1}{2}\left\{ \frac{1}{2L_x}\int\limits_{-L_x}^{L_x}\frac{\mathrm{d}x}{\sqrt{1+[f'(x)]^2}} \right\} n_2^2 S_0 + \frac{1}{2}A\left\{ \frac{1}{2L_x}\int\limits_{-L_x}^{L_x}\frac{1-[f'(x)]^2}{\sqrt{1+[f'(x)]^2}}\mathrm{d}x \right\} S_0 \\ & + \frac{1}{2}A\left\{ \frac{1}{2L_x}\int\limits_{-L_x}^{L_x}\frac{2f'(x)}{\sqrt{1+[f'(x)]^2}}\mathrm{d}x \right\} n_1n_3S_0 - \frac{1}{2}A\left\{ \frac{1}{2L_x}\int\limits_{-L_x}^{L_x}\frac{\mathrm{d}x}{\sqrt{1+[f'(x)]^2}} \right\} S_0. \end{aligned} \tag{13}$$

There are four terms on the right-hand side of Eq. (13), the third term is zero because $f(x)$ is a periodic function, the fourth term is a constant. Defining two parameters p and q as

$$p = \frac{1}{2L_x}\int\limits_{-L_x}^{L_x}\frac{\mathrm{d}x}{\sqrt{1+[f'(x)]^2}}, \tag{14}$$

$$q = \frac{1}{2L_x}\int\limits_{-L_x}^{L_x}\sqrt{1+[f'(x)]^2}\mathrm{d}x, \tag{15}$$

if the constant term in Eq.(13) is ignored, the anchoring energy per unit area of the projected plane of the grating surface is

$$g_s^{(1)} = \frac{1}{2}Ap(\boldsymbol{n}\cdot\boldsymbol{j})^2 + \frac{1}{2}A(2p-q)(\boldsymbol{n}\cdot\boldsymbol{i})^2. \tag{16}$$

ii) From Eq.(8), we obtain

$$G_s^{(1)} = \iint\limits_S \left\{ \frac{1}{2}A_1n_2^2 + \frac{1}{2}A_2\frac{1}{1+[f'(x)]^2}[n_1+f'(x)n_3]^2 \right\} \mathrm{d}S, \tag{17}$$

then

$$g_s^{(1)} = \frac{1}{2}[A_1q - A_2(q-p)](\boldsymbol{n}\cdot\boldsymbol{j})^2 + \frac{1}{2}A_2(2p-q)(\boldsymbol{n}\cdot\boldsymbol{i})^2. \tag{18}$$

Equations (16) and (18) may be expressed uniformly as

$$g_s^{(1)} = \frac{1}{2}w_1(\boldsymbol{n}\cdot\boldsymbol{j})^2 + \frac{1}{2}w_2(\boldsymbol{n}\cdot\boldsymbol{i})^2, \tag{19}$$

where w_1 and w_2 can be expressed uniformly as $w_1 = A_1 q - A_2(q-p)$, $w_2 = A_2(2p-q)$ and for case i) $A_1 = A_2 = A$. Considering that an interval of $2L_x$ contains $\dfrac{2L_x}{\lambda}$ cycles in total, and introducing a transformation $t = \dfrac{2\pi}{\lambda}x$, Eqs.(14) and (15) can be re-expressed in a more convenient form as follows:

$$p = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{\mathrm{d}t}{\sqrt{1+\left[f'\left(\dfrac{\lambda}{2\pi}t\right)\right]^2}}, \tag{20}$$

$$q = \frac{1}{2\pi}\int_{-\pi}^{\pi} \sqrt{1+\left[f'\left(\frac{\lambda}{2\pi}t\right)\right]^2}\,\mathrm{d}t, \tag{21}$$

where $f'\left(\dfrac{\lambda}{2\pi}t\right) = \dfrac{\mathrm{d}f(x)}{\mathrm{d}x}\Big|_{x=\frac{\lambda}{2\pi}t} = -\left(2\pi\dfrac{\delta}{\lambda}\right)^2 \sin t$. We see that both p and q are dependent on δ and λ.

Secondly, we consider the second mechanism. Berreman[11,12] has given the expression of this increased elastic strain energy per unit volume g_v. Supposing that the angle between director $\boldsymbol{n}$ and grooves (or channels, which are parallel to the oy-axis) is θ_y and adopting our symbols used in this paper, g_v can be written as

$$g_v = 8\pi^4\bar{k}(\delta^2/\lambda^2)\sin^2\theta_y \exp(-4\pi z/\lambda), \tag{22}$$

where $\bar{k}$ is the average of elastic constants. Then the equivalent anchoring energy per unit area of the projected plane of the grating surface is

$$g_s^{(2)} = \int_0^h g_v \mathrm{d}z, \tag{23}$$

where h is the thickness of the elastic strain layer. If $h \gg \lambda/(4\pi)$, then

$$g_s^{(2)} = 2\pi^3\bar{k}\frac{\delta^2}{\lambda^3}\sin^2\theta_y. \tag{24}$$

This result is the same as that in Ref.[10], where they refer to $2\pi^3\bar{k}\dfrac{\theta^2}{\lambda^3}$ as a maximum twist torque. From this result, we can obtain the equivalent anchoring energy originating from this mechanism. Let

$$F = 4\pi^3\bar{k}\frac{\theta^2}{\lambda^3}, \tag{25}$$

then

$$g_s^{(2)} = -\frac{1}{2}F(\boldsymbol{n}\cdot\boldsymbol{j})^2. \tag{26}$$

Substituting Eqs.(19) and (26) into Eq.(4), g_s can be written as

$$g_s = \frac{1}{2}W_1(\boldsymbol{n}\cdot\boldsymbol{j})^2 + \frac{1}{2}W_2(\boldsymbol{n}\cdot\boldsymbol{i})^2, \tag{27}$$

where $W_1 = w_1 - F$ and $W_2 = w_2$.

3. Anchoring properties of grating surface

Anchoring properties of substrate with a grating surface can be described by the strength and the direction of equivalent anchoring energy. Formally, the equivalent anchoring energy formula we have deduced is the same as the expression proposed in Refs.[6] and [7]. However, W_1 and W_2 are a function of δ and λ. For example in case i) described by Eq.(16), we have

$$W_1 = Ap - F, \quad W_2 = A(2p-q). \tag{28}$$

The dependences of $W_i/A(i=1,2)$ on δ/λ for case i) with different anchoring strengths A are shown in Fig.2, and the dependences of $W_i/A_1(i=1,2)$ on δ/λ for case ii) with different anchoring strengths A_1 are shown in Fig.3. The material parameters of liquid crystals are $k_{11} = 16.7\,\mathrm{pN}$, $k_{22} = 8.0\,\mathrm{pN}$, $\bar{k} = \sqrt{k_{11}\cdot k_{22}}$, and the pitch of a grating surface is $\lambda = 1\,\mu\mathrm{m}$.

From Fig.2 and Fig.3 we can see that W_1 and W_2 decrease and can change from positive to negative with the increase of δ/λ for a certain anchoring strength, and the smaller value of δ/λ when W_i/A or W_i/A_1 equals zero becomes bigger with the increase of anchoring strength. We also can see that for weak anchoring strengths the influence of δ/λ on W_1 is more prominent (Fig.2(a) and Fig.3(a)) and for strong anchoring strengths the influence of δ/λ on W_2 is more pronounced (Fig.2(c) and Fig.3(c)).

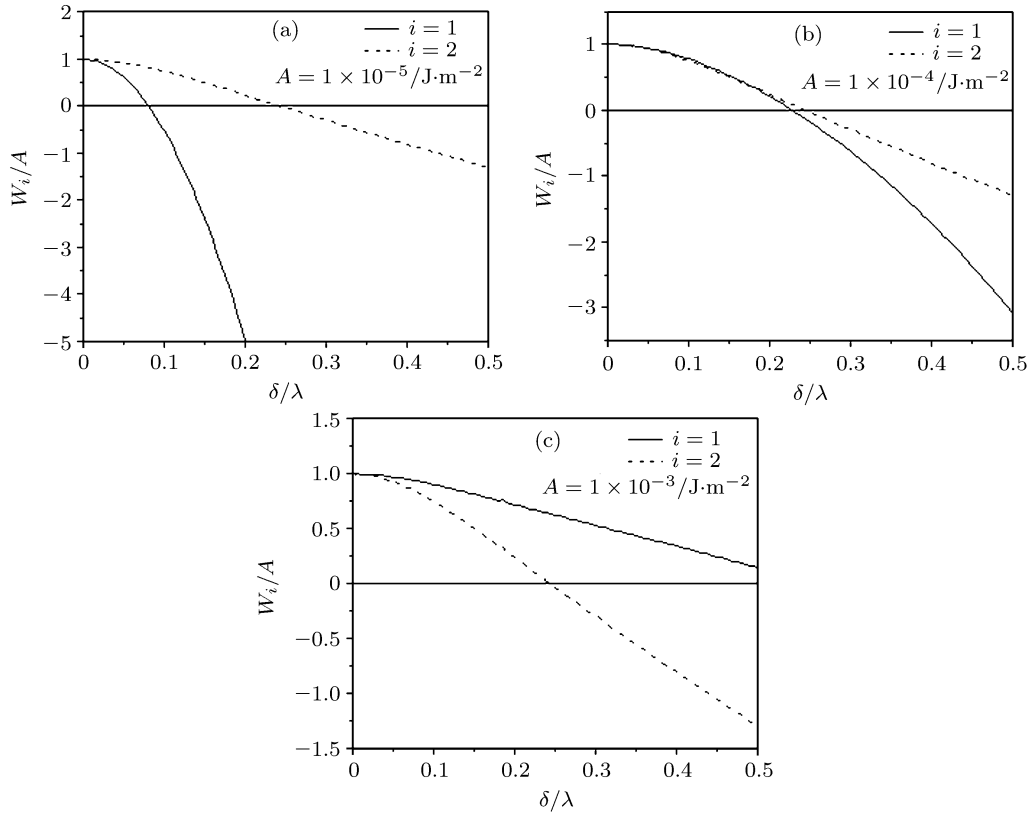


Fig.2. Dependences of $W_i/A(i = 1, 2)$ on δ/λ for case i) with different anchoring strengths A. The material parameters of liquid crystals are $k_{11} = 16.7\,\mathrm{pN}$, $k_{22} = 8.0\,\mathrm{pN}$, $\bar{k} = \sqrt{k_{11} \cdot k_{22}}$, and the pitch of a grating surface is $\lambda = 1\,\mu\mathrm{m}$.

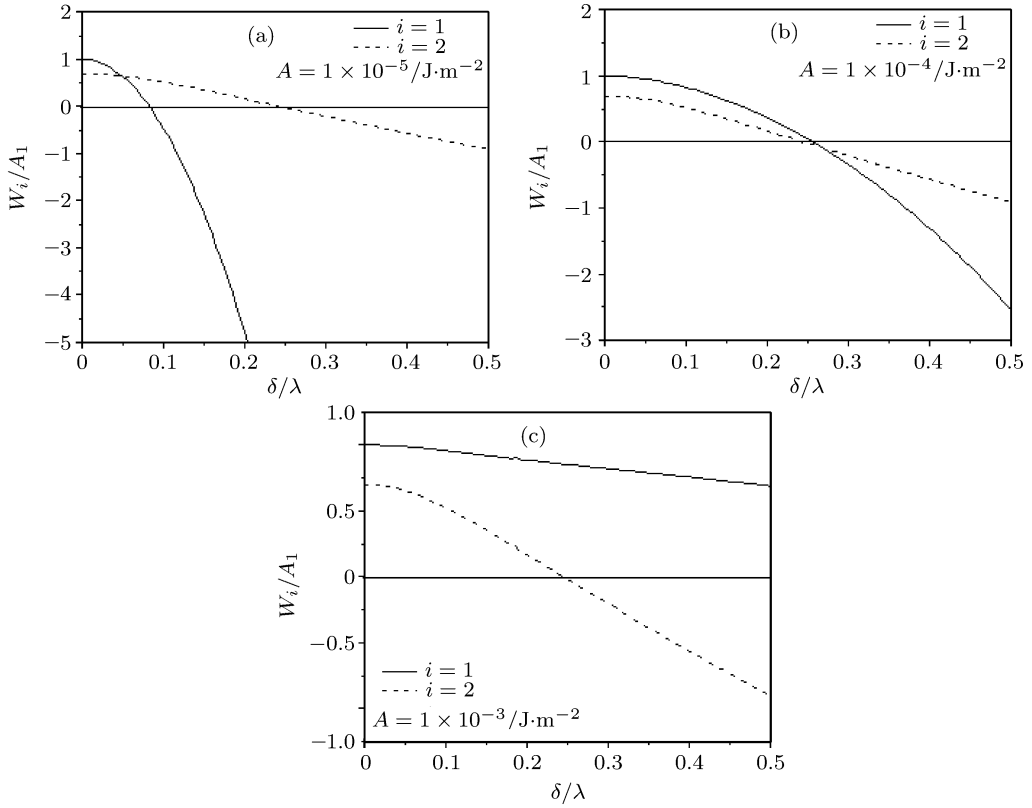


Fig.3. Dependences of $W_i/A_1(i = 1, 2)$ on δ/λ for case ii) with different anchoring strengths A_1. The material parameters of liquid crystals are $k_{11} = 16.7\,\mathrm{pN}$, $k_{22} = 8.0\,\mathrm{pN}$, $\bar{k} = \sqrt{k_{11} \cdot k_{22}}$, and the pitch of a grating surface is $\lambda = 1\,\mu\mathrm{m}$.

Moreover, the easy direction of anchoring is dependent on δ and λ also. The easy direction of equivalent anchoring is defined as a certain value of the direction of director $\boldsymbol{n}$, which makes g_s minimum. Because of $\boldsymbol{n} = (\cos\theta\cos\phi, \cos\theta\sin\phi, \sin\theta)$, Eq.(27) can be re-expressed as

$$g_s = \frac{1}{2}W_1\cos^2\theta\sin^2\phi + \frac{1}{2}W_2\cos^2\theta\cos^2\phi. \quad (29)$$

The tilt angle θ and azimuthal angle ϕ of easy direction satisfy the conditions as follows:

$$\frac{\partial g_s}{\partial\theta} = -\frac{1}{2}(W_1\sin^2\phi + W_2\cos^2\phi)\sin 2\theta = 0, \quad (30)$$

$$\frac{\partial g_s}{\partial\phi} = -\frac{1}{2}(W_2 - W_1)\cos^2\theta\sin 2\phi = 0. \quad (31)$$

The solutions are $\theta = 0, \pi/2$ and $\phi = 0, \pi/2$. There are four combinations for θ and ϕ, i.e. there are four solutions. According to Eq.(29), we obtain four possibilities as follows:

(a) Both W_1 and W_2 are larger than zero. In this case, $\theta = \dfrac{\pi}{2}$, ϕ is arbitrary, the easy direction is $\boldsymbol{k}$.

(b) Both W_1 and W_2 are less than zero. If $|W_1| > |W_2|$, then $\theta = 0$, $\phi = \dfrac{\pi}{2}$, the easy direction is $\boldsymbol{j}$; if $|W_1| < |W_2|$, then $\theta = 0$, $\phi = 0$, the easy direction is $\boldsymbol{i}$.

(c) $W_1 > 0$ and $W_2 < 0$. In this case, $\theta = 0$, $\phi = 0$, the easy direction is $\boldsymbol{i}$.

(d) $W_1 < 0$ and $W_2 > 0$. In this case, $\theta = 0$, $\phi = \dfrac{\pi}{2}$, the easy direction is $\boldsymbol{j}$.

From the above analysis we can know that this kind of variation in the strength of equivalent anchoring energy will directly affect the direction of equivalent anchoring energy, which can change this display mode from homogeneous cell to hybrid aligned nematic cell, vertical aligned cell or twist nematic cell. As a result, one can realize different display modes by choosing an appropriate value of δ/λ.

4. Discussion

To gain a better effect in liquid crystal display, the substrate anchoring action is very important, especially for the particular substrates such as the substrate with a grating surface. This kind of substrate with a grating surface can be used to fabricate zenithal bistable devices,[13−18] which have enormous potential for application and would become a new mode of liquid crystal display in the next generation.[10]

Applying our formula, one can theoretically analyse the anchoring properties of substrates with a grating surface. Additionally, one can analyse some characters of liquid crystal cell such as the distribution of NLC director, Fréedericksz transition, the transmittance, the response time and so on. Therefore, it can provide a certain guidance for liquid crystal technology.

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