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Equivalent anchoring energy formula of a NLC on a grating surface and VCT effect

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The voltage-controlled twist (VCT) effect shows that a grating surface, with its particular anchoring properties, has the potential to become a new surface anchoring for liquid crystal devices. In order to describe these properties an equivalent anchoring energy is introduced. The alignment of a nematic liquid crystal (NLC) on such a grating originates from two mechanisms, so each produces a term in the equivalent anchoring energy. One is the interaction potential between NLC molecules and the molecules on the substrate surface, from which we derive the expression of the corresponding term. The other is the increased elastic strain energy, for which we adopt the result of Berreman. The equivalent anchoring energy obtained is a function of pitch λ and amplitude δ of the grating surface. Both the corresponding strength parameter and the easy direction are functions of λ and δ. The hybrid aligned nematic cell proposed by. Bryan-Brown *et al.* is studied by the use of our formula, and the distribution of the director, the saturation state and the saturation voltage are calculated in detail. The results are consistent with experimental data, especially the values of λ and δ. The VCT effect can therefore be explained.

1. Introduction

Bryan-Brown *et al.* [1] discovered the voltage-controlled twist (VCT) effect in a hybrid aligned nematic cell (HAN cell). This effect is attributed to the particular substrate with a grating surface, which is a mono-grating of suitable pitch and amplitude coated with a homeotropic layer. The grating surface is used to manufacture (ZBD) devices and is called a ZBD surface [2–9]. Bryan-Brown and co-workers have predicted that this kind of device has great applications potential and will become a new mode for next generation liquid crystal displays (LCDs).

Anchoring effects in a NLC cell can usually be studied by the analytical method according to NLC continuum theory. However, it is difficult to apply this to the HAN cell proposed in [1], because the grating surface is a macroscopic complex curved surface, and the tilt angle θ and twist angle ϕ of the director are functions of two coordinate values x and z, i.e. $\theta=\theta(x, z)$, $\phi=\phi(x, z)$. Therefore, we should solve the non-linear differential equation of the two-dimensional functions $\theta(x, z)$ and $\phi(x, z)$ under curved surface boundary conditions. This is a difficult and troublesome task.

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In order to remove this difficulty, in this paper we introduce the concept of equivalent anchoring energy. The projected plane of a grating surface is a flat plane and is used to replace the macroscopic curved surface, i.e. the grating surface. We derive an expression for anchoring energy per unit area of this projected plane. This expression is termed the formula for equivalent anchoring energy. By using this formula one can solve the equation of a NLC director under flat plane boundary conditions. Thus the anchoring property of a grating surface is described by the formula for equivalent anchoring energy.

Because the grating surface is a mono-grating of suitable pitch λ and amplitude δ, with a homeotropic layer, the NLC alignment originates from two mechanisms and so the anchoring energy consists of two parts. One is the interaction potential between NLC molecules and molecules of the substrate surface [10]. The other is elastic strain energy in the NLC bulk that would be increased if NLC molecules were aligned by the surface but were not parallel to the groove (or channel) direction [1, 11]. For the first mechanism, we start with the ordinary anchoring energy density, whose integral over the grating surface is the total anchoring energy. We prove that it can be re-expressed as an integral over the projected plane of the grating surface, i.e. a flat plane integral. Then we obtain the anchoring energy per

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unit area of the projected plane for this part, which is denoted by $g_s^{(1)}$. For the second mechanism, we adopt the result of Berreman [11, 12]. Following de Gennes [13] and Bryan-Brown [1], this part of the equivalent anchoring energy is denoted by $g_s^{(2)}$. Then the total anchoring energy density is

$$g_s = g_s^{(1)} + g_s^{(2)} \qquad (1)$$

where both $g_s^{(1)}$ and $g_s^{(2)}$ are functions of λ and δ. Then we obtain the expression of equivalent anchoring energy density.

The definite expression for g_s is determined by the geometry of the grating surface. If the grating surface is cosinoidal (or sinoidal), the expression has similar form as adopted in [14, 15] or discussed in [10], i.e. there are two terms and two anchoring strength parameters W_1 and W_2 respectively; both W_1 and W_2 are functions of λ and δ. Moreover, the easy direction is also related to λ and δ.

As an important application of our formula, we study the VCT effect. By using the equivalent anchoring energy g_s, θ and ϕ are functions of one value of coordinate z, and both boundaries of the cell can be seen as a flat plane. The Gibbs free energy for this HAN cell under an applied voltage is to be written. For a given voltage, the electric field **E** varies with position in the cell, so a variational calculation must be made under the condition that the voltage is given and definite. Adopting a proper variational approach [16, 17], the differential equation and boundary condition of θ and ϕ will be derived.

We calculate the distribution of tilt angle θ and twist angle ϕ of director for a given voltage, the saturation voltage and the corresponding twist angle ϕ_0. All these quantities are functions of λ and δ. The relationship between the VCT effect and geometrical properties of the grating surface can be understood from these results. Thus our formula for equivalent anchoring energy may be checked by this effect.

Zhao *et al.* [14, 15] have studied the VCT effect using their own anchoring energy formula; however, in their theory the grating surface boundary is seen as a flat plane and the results obtained do not relate to the geometrical properties of the grating surface.

2. Equivalent anchoring energy formula

In this section, we study the anchoring energy corresponding to the grating surface. The geometrical configuration of the grating surface is shown in figure 1. The grating long narrow channels are parallel to the *oy*-axis, and the intersectant line between the grating surface and the *xz*-plane is a periodic curve. The equation of the grating surface can be written as

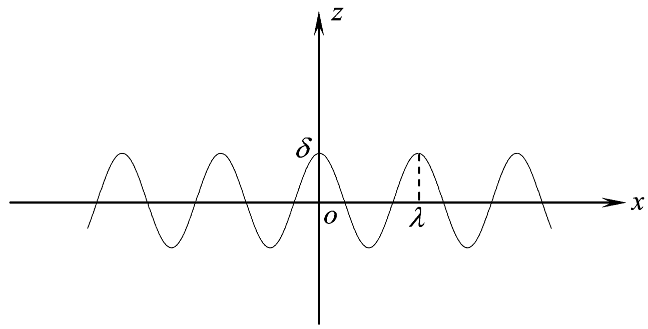

Figure 1. The intersectant line between grating surface and *xz*-plane; δ is the amplitude, λ the pitch.

$$z = f(x) \qquad (2a)$$

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 δ_2, δ_3 ...... are very small compared with δ_1, then the expression can be simplified to

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

This is a cosinoidal surface (or sinoidal surface), such as that described in [1], where the pitch λ is the distance between two adjacent channels, and δ is the amplitude which is the depth of channel. So the geometry of the grating surface can be described by the two parameters λ and δ.

We next discuss the anchoring energy. Since the alignment of a NLC on the grating surface originates from two mechanisms, the anchoring energy consists of two parts. One originates from the interaction potential between NLC molecules and the molecules of the substrate surface, the other originates from the increased elastic strain energy.

Let us consider the first mechanism, mentioned earlier. Suppose that the grating surface area element is dS. According to [10], anchoring energy can be seen as the sum of the interaction potential between surface molecules and liquid crystal molecules, and is related to the equivalent orientation **e** of surface molecules on the substrate surface. Suppose that the unit vector normal to dS is **v**, as stated by [10], there are two possibilities for homeotropic anchoring.

(i) If **e** is along **v** and the interaction potential is negative, the anchoring energy of dS will be

$$-\frac{1}{2} A(\mathbf{n}\cdot\mathbf{v})^2 \mathrm{d}S. \qquad (3)$$

(ii) If **e** is along the direction of the *oy*-axis, i.e. parallel to the groove (or channel), and the interaction potential is positive, the anchoring energy of dS will be

$$\left\{\frac{1}{2}A_1(\mathbf{n}\cdot\mathbf{j})^2+\frac{1}{2}A_2(\mathbf{n}\cdot\mathbf{j}\times\mathbf{v})^2\right\}\mathrm{d}S \tag{4}$$

where **i**, **j** and **k** are basic vectors along the *ox*-, *oy* and *oz*-axis, respectively, and A, A_1, A_2 are parameters of the anchoring strength and greater than zero. Then we shall discuss these two cases separately

(i) *The interaction potential is negative*. From equation (3), we obtain

$$g_s^{(1)}=\iint_S\left\{-\frac{A}{2}(\mathbf{n}\cdot\mathbf{v})^2\right\}\mathrm{d}S \tag{5}$$

where S is the grating surface. An expression for **v** can be obtained from equation (2a):

$$\mathbf{v}=\frac{1}{\left\{1+[f'(x)]^2\right\}^{\frac{1}{2}}}[-f'(x)\mathbf{i}+\mathbf{k}] \tag{6}$$

where $f'(x)=\frac{\mathrm{d}f(x)}{\mathrm{d}x}$ and for a cosinoidal surface, equation (2 b), $f'(x)=-2\pi\frac{\delta}{\lambda}\sin\left(\frac{2\pi}{\lambda}x\right)$. Considering $\mathbf{n}=n_1\mathbf{i}+n_2\mathbf{j}+n_3\mathbf{k}$, equation (5) can be rewritten as

$$g_s^{(1)}=-\frac{A}{2}\iint_S\frac{1}{1+[f'(x)]^2}[-n_1f'(x)+n_3]^2\mathrm{d}S. \tag{7}$$

Considering $n_3^2=1-n_1^2-n_2^2$ and $v_3\,\mathrm{d}S=\mathrm{d}x\mathrm{d}y$, where $v_3=\frac{1}{\left\{1+[f'(x)]^2\right\}^{\frac{1}{2}}}$, equation (7) becomes

$$g_s^{(1)}=\frac{A}{2}\iint_{S_0}\left[n_2^2\frac{1}{\left\{1+[f'(x)]^2\right\}^{\frac{1}{2}}}+n_1^2\frac{1-[f'(x)]^2}{\left\{1+[f'(x)]^2\right\}^{\frac{1}{2}}}+2n_1n_3\frac{f'(x)}{\left\{1+[f'(x)]^2\right\}^{\frac{1}{2}}}-\frac{1}{\left\{1+[f'(x)]^2\right\}^{\frac{1}{2}}}\right]\mathrm{d}x\,\mathrm{d}y \tag{8}$$

where S_0 denotes the area of the projected plane of the grating surface on the *xy*-plane.

If the variation of **n** is very small in the interval $|\Delta z\leqslant\delta|$, equation (8) can be approximated as

$$\begin{aligned}g_s^{(1)}=&\frac{1}{2}A\left\{\frac{1}{2L_x}\int_{-L_x}^{L_x}\frac{\mathrm{d}x}{\left\{1+[f'(x)]^2\right\}^{\frac{1}{2}}}\right\}n_2^2S_0+\\&\frac{1}{2}A\left\{\frac{1}{2L_x}\int_{-L_x}^{L_x}\frac{1-[f'(x)]^2}{\left\{1+[f'(x)]^2\right\}^{\frac{1}{2}}}\mathrm{d}x\right\}S_0+\\&\frac{1}{2}A\left\{\frac{1}{2L_x}\int_{-L_x}^{L_x}\frac{2f'(x)}{\left\{1+[f'(x)]^2\right\}^{\frac{1}{2}}}\mathrm{d}x\right\}n_1n_3S_0-\\&\frac{1}{2}A\left\{\frac{1}{2L_x}\int_{-L_x}^{L_x}\frac{\mathrm{d}x}{\left\{1+[f'(x)]^2\right\}^{\frac{1}{2}}}\right\}S_0\end{aligned} \tag{9}$$

where $S_0=(2L_x)\times(2L_y)$; L_x and L_y denote the length and breadth of the liquid crystal cell, respectively. There are four terms in equation (9), the third term is zero because $f(x)$ is a periodic function, the fourth term is a constant. In order to simplify equation (9), we define two parameters p and q

$$p=\frac{1}{2L_x}\int_{-L_x}^{L_x}\frac{\mathrm{d}x}{\left\{1+[f'(x)]^2\right\}^{\frac{1}{2}}} \tag{10}$$

$$p=\frac{1}{2L_x}\int_{-L_x}^{L_x}\left\{1+[f'(x)]^2\right\}^{\frac{1}{2}}\mathrm{d}x. \tag{11}$$

If the constant term in equation (9) is ignored, the anchoring energy per unit area of the projected plane of the grating surface is

$$g_s^{(1)}=\frac{1}{2}Ap(\mathbf{n}\cdot\mathbf{j})^2+\frac{1}{2}A(2p-q)(\mathbf{n}\cdot\mathbf{i})^2. \tag{12}$$

(ii) ***The interaction potential is positive***. From equation (4), we obtain

$$g_s^{(1)}=\iint_S\left\{\frac{1}{2}A_1n_2^2+\frac{1}{2}A_2\frac{1}{1+[f'(x)]^2}[n_1+f'(x)n_3]^2\right\}\mathrm{d}S \tag{13}$$

then

$$g_s^{(1)}=\frac{1}{2}[A_1q-A_2(q-p)](\mathbf{n}\cdot\mathbf{j})^2+\frac{1}{2}A_2(2p-q)(\mathbf{n}\cdot\mathbf{i})^2. \tag{14}$$

Equation (12) and (14) may be expressed uniformly as

$$g_s^{(1)} = \frac{1}{2} w_1 (\mathbf{n}\cdot\mathbf{j})^2 + \frac{1}{2} w_2 (\mathbf{n}\cdot\mathbf{i})^2 \tag{15}$$

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 $2L_x/\lambda$ periods in all, and introducing a transformation $t=2\pi x/\lambda$, equations (10) and (11) can be re-expressed in the more convenient form

$$p = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\mathrm{d}t}{\left\{1+\left[f'\left(\frac{\lambda}{2\pi}t\right)\right]^2\right\}^{\frac{1}{2}}} \tag{16}$$

$$q = \frac{1}{2\pi} \int_{-\pi}^{\pi} \left\{1+\left[f'\left(\frac{\lambda}{2\pi}t\right)\right]^2\right\}^{\frac{1}{2}} \mathrm{d}t \tag{17}$$

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

Now, let us turn to the second mechanism. Berreman [11, 12] has given the expression of the increased elastic strain energy per unit volume g_v. We define the angle between the director $\mathbf{n}$ and grooves (or channels, parallel to the oy-axis) as θ_y and adopt the symbols used in this paper; g_v can be written as

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

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

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

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

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

This result is same as in [1], where they consider $2\pi^3 k \frac{\delta^2}{\lambda^3}$ as the maximum twist torque. From this result, we can obtain the equivalent anchoring energy for this mechanism. Suppose that

$$F = 4\pi^3 \bar{k} \frac{\delta^2}{\lambda^3} \tag{18}$$

then

$$g_s^{(2)} = -\frac{1}{2} F (\mathbf{n}\cdot\mathbf{j})^2. \tag{19}$$

Substituting equations (15) and (19) into equation (1), g_s can be written as

$$\begin{aligned} g_s &= \frac{1}{2}(w_1 - F)(\mathbf{n}\cdot\mathbf{j})^2 + \frac{1}{2} w_2 (\mathbf{n}\cdot\mathbf{i})^2 \\ &= \frac{1}{2} W_1 (\mathbf{n}\cdot\mathbf{j})^2 + \frac{1}{2} W_2 (\mathbf{n}\cdot\mathbf{i})^2 \end{aligned} \tag{20}$$

where $W_1=w_1-F$ and $W_2=w_2$. Formally, it is the same as the expressions proposed in [10] and [15]. However, W_1 and W_2 are functions of δ and λ. For example, in case (i) described by equation (12), we have

$$W_1 = Ap - F,\ W_2 = A(2p-q). \tag{21}$$

Moreover, the easy direction of anchoring depends on λ and δ. The easy direction of equivalent anchoring, which makes g_s minimum, is defined as a certain value of the direction of director $\mathbf{n}$. Because $\mathbf{n}=(\cos\theta\cos\phi, \cos\theta\sin\phi, \sin\theta)$, equation (20) can be re-expressed as

$$g_s = \frac{1}{2} W_1 \cos^2\theta \sin^2\phi + \frac{1}{2} W_2 \cos^2\theta\cos^2\phi. \tag{23}$$

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

$$\frac{\partial g_s}{\partial\theta} = -\frac{1}{2}\left(W_1 \sin^2\phi + W_2\cos^2\phi\right)\sin 2\theta = 0 \tag{24a}$$

$$\frac{\partial g_s}{\partial\phi} = -\frac{1}{2}(W_2 - W_1)\cos^2\theta \sin 2\phi = 0. \tag{24b}$$

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 equation (23), we obtain four possibilities as follows:

(a) If both W_1 and W_2, are larger than zero, then $\theta=\frac{\pi}{2}$, ϕ is arbitrary, the easy direction is $\mathbf{k}$.
(b) If both W_1 and W_2 are less than zero and $|W_1|>|W_2|$, then $\theta=0$, $\phi=\frac{\pi}{2}$, the easy direction is $\mathbf{j}$; if both W_1 and W_2 are less than zero and $|W_1|<|W_2|$, then $\theta=0$, $\phi=0$, the easy direction is $\mathbf{i}$.
(c) If $W_1>0$ and $W_2<0$, then $\theta=0$, $\phi=0$, the easy direction is $\mathbf{i}$.
(d) If $W_1<0$ and $W_2>0$, then $\theta=0$, $\phi=\frac{\pi}{2}$, the easy direction is $\mathbf{j}$.

Because the values of W_1 and W_2 are related to the values of λ and δ, the easy direction is also related to λ and δ. So we can conclude that the parameters of equivalent anchoring energy W_1 and W_2 and the easy direction of anchoring depend on of λ and δ. Variations of $W_i/A(i=1, 2)$ and $W_i/A_1(i=1,2)$ versus δ/λ for fixed λ and $\bar{k}$ are shown in figure 2. We see that W_1 and W_2 decrease and can change from positive to negative as δ/λ increases. For case (i), when $\delta/\lambda<0.083$, $W_1>0$, $W_2>0$, the easy direction is **k**; when $0.083<\delta/\lambda<0.243$, $W_1<0$, $W_2>0$, the easy direction is **j**. For case (ii), when $\delta/\lambda<0.113$, $W_1>0$, $W_2>0$, the easy direction is **k**; when $0.113<\delta/\lambda<0.243$, $W_1<0$, $W_2>0$, the easy direction is **j**.

3. Distribution of the director in a HAN cell

We now discuss the VCT effect. A HAN cell described in [1] is shown in figure 3. Two substrates are placed at $z=0$ and $z=1$ respectively. The upper substrate has a plane surface with strong homogenouse anchoring, while lower substrate has a grating surface with weak homeotropic anchoring. The grating surface is described by $z=\delta\cos\left(\frac{2\pi}{\lambda}x\right)$. A voltage U is applied to this cell.

The Gibbs free energy consists of three parts. By using the equivalent anchoring energy formula, they can be expressed as:

(1) Frank elastic free energy

$$G_{\text{elastic}}=S_0\int_0^l\left\{\frac{1}{2}f(\theta)\left(\frac{d\theta}{dz}\right)^2+\frac{1}{2}h(\theta)\left(\frac{d\phi}{dz}\right)^2\right\}dz \quad (25)$$

where $f(\theta)=k_{11}\cos^2\theta+k_{33}\sin^2\theta$, $h(\theta)=\cos^2\theta(k_{22}\cos^2\theta+k_{33}\sin^2\theta)$ [18].

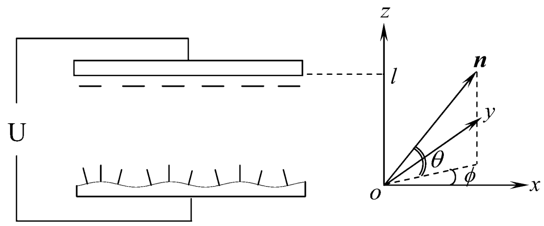

Figure 3. Sketch map of HAN cell and coordinate system.

(2) The dielectric free energy. It can be expressed [17] approximately as

$$G_{\text{electric}}=S_0\int_0^l\left\{-\frac{1}{2}\frac{D_3^2}{j(\theta)}\right\}dz \quad (26)$$

where $j(\theta)=\varepsilon_\perp+\Delta\varepsilon\sin^2\theta$; $\Delta\varepsilon=\varepsilon_{//}-\varepsilon_\perp$ is the dielectric anisotropy of the liquid crystal material; and

$$D_3=\frac{U}{\int_0^l\frac{dz}{j(\theta)}}. \quad (27)$$

(3) Surface free energy, i.e. anchoring energy. At $z=0$ this is written as

$$G_{\text{surface}}=S_0\left[\frac{1}{2}\cos^2\theta_0\left(W_1\sin^2\phi_0+W_2\cos^2\phi_0\right)\right] \quad (28)$$

and at $z=l$ it can be replaced by

$$\theta_l=0,\quad \phi_t=0. \quad (29)$$

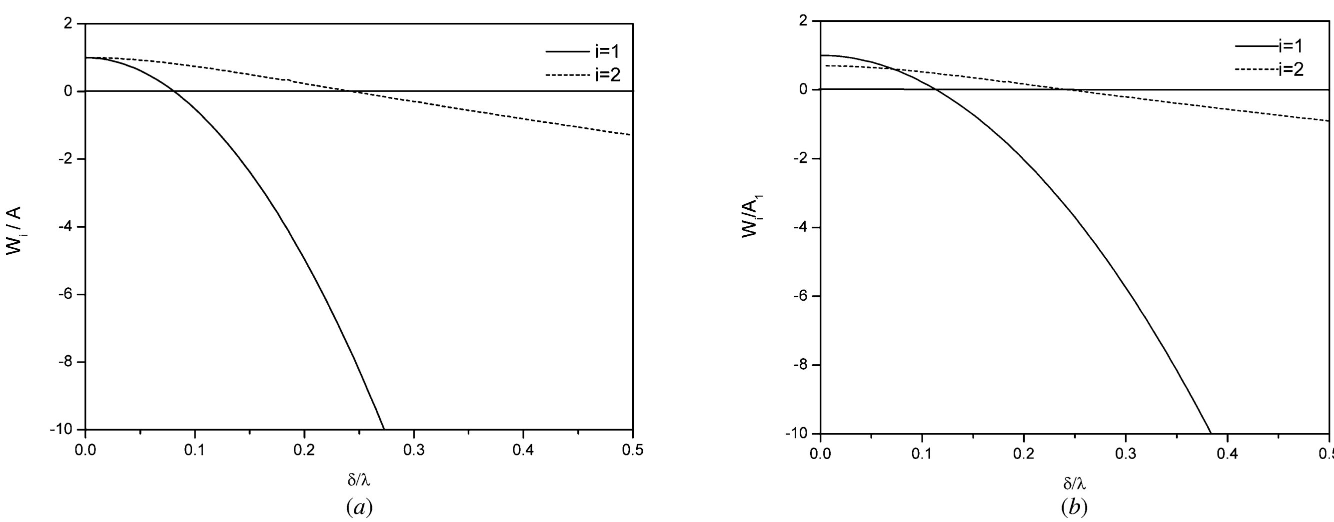

Figure 2. Variations of $W_i/A(i=1,2)$ and $W_i/A_1(i=1,2)$ versus δ/λ. (*a*) For case (i), the interaction potential between surface molecules and liquid crystal molecules is negative, $\lambda=1\,\mu m$, $\bar{k}=11.6\,pN$; (*b*) for case (ii), the interaction potential between surface molecules and liquid crystal molecules is positive, $A_2/A_1=0.7$, $\lambda=1\,\mu m$, $\bar{k}=11.6\,pN$.

The total Gibbs free energy is

$$G=G_{\text{elastic}}+G_{\text{electric}}+G_{\text{surface}}. \tag{30}$$

Now we calculate the variation of G for a given voltage by applying the method described in [16, 17]. Suppose

$$\theta=\overline{\theta}+\alpha\xi \tag{31a}$$

$$\phi=\overline{\phi}+\beta\eta \tag{31b}$$

where $\bar{\theta}$ and $\bar{\phi}$ for minimum G are functions of z, ξ and η are arbitrary functions of z, and α and β are common variables. Substituting equations (31 *a*) and (31 *b*) into (30), G becomes a function of α and β. From $\frac{\partial G}{\partial\alpha}\Big|_{\substack{\alpha=0\\ \beta=0}}=0$ and $\frac{\partial G}{\partial\beta}\Big|_{\substack{\alpha=0\\ \beta=0}}=0$ we can obtain equations for $\theta(z)$ and $\phi(z)$

$$\frac{1}{2}\frac{\mathrm{d}f(\theta)}{\mathrm{d}\theta}\theta'^2-\frac{\mathrm{d}}{\mathrm{d}z}[f(\theta)\theta']+\frac{1}{2}\frac{\mathrm{d}h(\theta)}{\mathrm{d}\theta}\phi'^2-\frac{1}{2}D_3^2\frac{\mathrm{d}}{\mathrm{d}\theta}\left[\frac{1}{j(\theta)}\right]=0 \tag{32}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}\left[h(\theta)\phi'\right]=0 \tag{33}$$

and boundary conditions for $z=0$

$$f(\theta_0)\theta_0'=-\frac{1}{2}\sin 2\theta_0\left(W_1\sin^2\phi_0+W_2\cos^2\phi_0\right) \tag{34}$$

$$h(\theta_0)\phi_0'=-\frac{1}{2}(W_2-W_1)\cos^2\theta_0\sin 2\phi_0. \tag{35}$$

From equations (33) and (35), we have

$$\phi'=\frac{C_1}{h(\theta)} \tag{36}$$

where

$$C_1=\frac{1}{2}(W_1-W_2)\cos^2\theta_0\sin 2\phi_0. \tag{37}$$

From equation (32), we have

$$f(\theta)\theta'^2+\frac{C_1^2}{h(\theta)}-\frac{D_3^2}{j(\theta)}=C \tag{38}$$

where

$$C=\frac{\sin^2 2\theta_0}{4f(\theta_0)}\left(W_1\sin^2\phi_0+W_2\cos^2\phi_0\right)^2-\frac{D_3^2}{j(\theta_0)}+\frac{C_1^2}{h(\theta_0)}. \tag{39}$$

Defining

$$\frac{\mathrm{d}\theta}{\mathrm{d}z}=-\frac{1}{N(\theta)} \tag{40}$$

from quations (38) and (39), we have

$$N(\theta)=\left\{\frac{f(\theta)}{C_1^2\left[\frac{1}{h(\theta_0)}-\frac{1}{h(\theta)}\right]-D_3^2\left[\frac{1}{j(\theta_0)}-\frac{1}{j(\theta)}\right]+\frac{\sin^2 2\theta_0}{4f(\theta_0)}\left(W_1\sin^2\phi_0+W_2\cos^2\phi_0\right)^2}\right\}^{\frac{1}{2}} \tag{41}$$

Then the solution of $\theta(z)$ can be expressed as

$$\int_0^{\theta(z)}N(\theta)\mathrm{d}\theta=l-z \tag{42}$$

and the solution of $\phi(z)$ is

$$\phi(z)=-\int_0^{\theta(z)}\frac{C_1}{h(\theta)}N(\theta)\mathrm{d}\theta. \tag{43}$$

Using equations (42) and (43), $\theta(z)$ and $\phi(z)$ can be calculated. At $z=0$, θ_0 and ϕ_0 satisfy

$$\int_0^{\theta_0}N(\theta)\mathrm{d}\theta=1 \tag{44}$$

$$\phi_0=-\int_0^{\theta_0}\frac{C_1}{h(\theta)}N(\theta)\mathrm{d}\theta. \tag{45}$$

In order to simplify $N(\theta)$, we define the reduced voltage u, the reduced anchoring strength α

$$u=U\Big/\pi\left(\frac{k_{11}}{|\Delta\varepsilon|}\right)^{\frac{1}{2}},\ \alpha=\frac{A_l l}{\pi k_{11}} \tag{46}$$

and parameters

$$\begin{aligned}&r=\frac{A_2}{A_1},\ \varepsilon'=\frac{\Delta\varepsilon}{\varepsilon_\perp},\ \mu=\frac{k_{33}-k_{11}}{k_{11}},\ \mu'=\frac{k_{33}-k_{22}}{k_{22}},\\ &W=\frac{W_2-W_1}{W_1}=\frac{rp-q+F/A_1}{rp-(r-1)q-F/A_1}.\end{aligned} \tag{47}$$

Some quantities in $N(\theta)$ can then be re-expressed as

$$\begin{aligned}&f(\theta)=k_{11}\left(1+\mu\sin^2\theta\right),\ h(\theta)=k_{22}\cos^2\theta\left(1+\mu\sin^2\theta\right),\\ &j(\theta)=\varepsilon_\perp\left(1+\varepsilon'\sin^2\theta\right),W_1=\frac{\pi k_{11}}{l}[rp-(r-1)q-F/A_1]\alpha,\\ &C_1=-\frac{1}{2}\frac{\pi k_{11}}{l}(rp-q+F/A_1)\alpha\cos^2\theta_0\sin 2\phi_0.\end{aligned} \tag{48}$$

Defining

$$S_\chi = 1 + \chi \sin^2 \theta,\ S_\chi^0 = 1 + \chi \sin^2 \theta_0 \tag{49}$$

where $\chi = \mu,\ \mu',\ \varepsilon'$ and

$$\left\langle \frac{1}{S_{\varepsilon'}} \right\rangle = \frac{1}{l} \int_0^l \frac{\mathrm{d}z}{S_{\varepsilon'}} \tag{50}$$

$$C_w^0 = 1 + W \cos^2 \phi_0 = 1 + \frac{rp - q + F/A_1}{rp - (r-1)q - G/A_1} \cos^2 \phi_0. \tag{51}$$

$N(\theta)$ can be expressed as

$$N(\theta) = \frac{1}{\pi} \left[\frac{S_\mu}{u^2 \frac{\sin^2\theta_0 - \sin^2\theta}{S_{\varepsilon'} S_{\varepsilon'}^0 \langle \frac{1}{S_{\varepsilon'}} \rangle^2} + \alpha^2 \cos^2\theta_0 \left\{ (rp - q + F/A_1)^2 \frac{k_{11}}{4k_{22}} \frac{\sin^2 2\phi_0 (\sin^2\theta_0 - \sin^2\theta)\left(S_{\mu'} + S_{\mu'}^0 - 1 - \mu'\right)}{\cos^2\theta S_{\mu'} S_{\mu'}^0} + [rp - (r-1)q - F/A_1]^2 \frac{\sin^2\theta_0}{S_\mu^0} \left(C_{\mathrm{w}}^0\right)^2 \right\}} \right]^{\frac{1}{2}} \tag{52}$$

From equation (52) we see that $N(\theta)$ is related to p and q; thus $\theta(z)$ and $\phi(z)$ are related to p and q, and are functions of λ and δ.

Figures 4 and 5 show the variation of tilt angle θ and twist angle ϕ with δ/λ, respectively. The material parameters used in the calculation are $k_{11} = 16.7$ pN, $k_{22} = 8.0$ pN, $k_{33} = 18.1$ pN, $\Delta\varepsilon = -4.2$ [14], and $A_2/A_1 = 0.7$, $\lambda = 1\,\mu$m. The applied voltage is $U = 0.5$ V. Both figures show a very marked change of θ and ϕ on the lower substrate when δ/λ changes from 0.11 to 0.12. This is because the easy direction on the lower substrate changes from **k** to **j**.

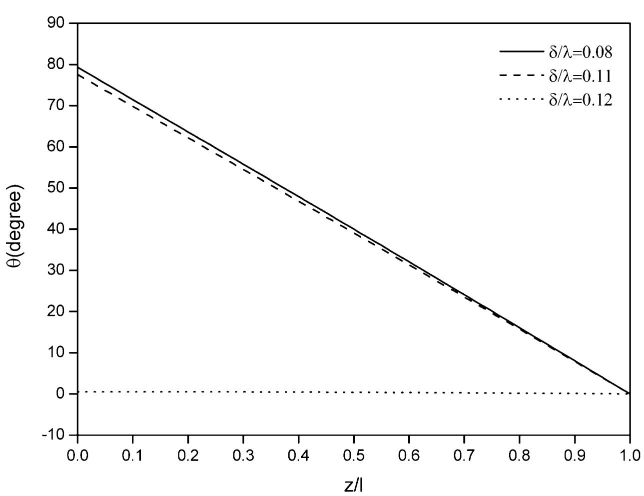

Figure 4. Variation of tilt angle θ with δ/λ. The material parameters used in the calculation are $k_{11} = 16.7$ pN, $k_{22} = 8.0$ pN, $k_{33} = 18.1$ pN, $\Delta\varepsilon = -4.2$, $r = 0.7$, $\lambda = 1\,\mu$m. The applied voltage is $U = 0.5$ V.

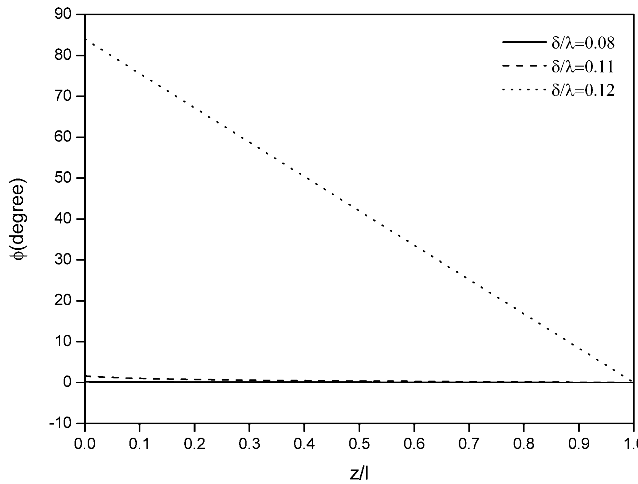

Figure 5. Variation of twist angle ϕ with δ/λ. Material parameters and applied voltage a for figure 4a $U = 0.5$ V.

4. Saturation state and saturation voltage

When the voltage applied to a HAN cell is larger than a critical value, the tilt angle θ of the director is zero throughout. This state is termed the saturation state, and the corresponding critical voltage is termed the saturation voltage, denoted as U_{sat}. We discuss the saturation state first. Because $\theta \equiv 0$, only $\phi(z)$ can be considered. From equations (45) and (36), we obtain

$$\phi_0 = \frac{\pi}{2} \frac{k_{11}}{k_{22}} (rp - q + F/A_1) \alpha \sin 2\phi_0 \tag{53}$$

and

$$\phi = \frac{\pi}{2} \frac{k_{11}}{k_{22}} \frac{rp - q + F/A_1}{l} \alpha \sin 2\phi_0 (l - z). \tag{54}$$

These results of numerical calculation for $\phi_0 \sim \delta/\lambda$ with different α are shown in Figure 6.

We now come to the saturation voltage. Using equations (52) and (44), the reduced saturation voltage can be calculated. Considering $\theta(z) \leqslant \theta_0$ for $0 \leqslant z \leqslant l$, we make a transformation of integral variable from θ to β, $\sin\theta = \sin\theta_0 \sin\beta$. With some simplifications, equation (44) can be rewritten as

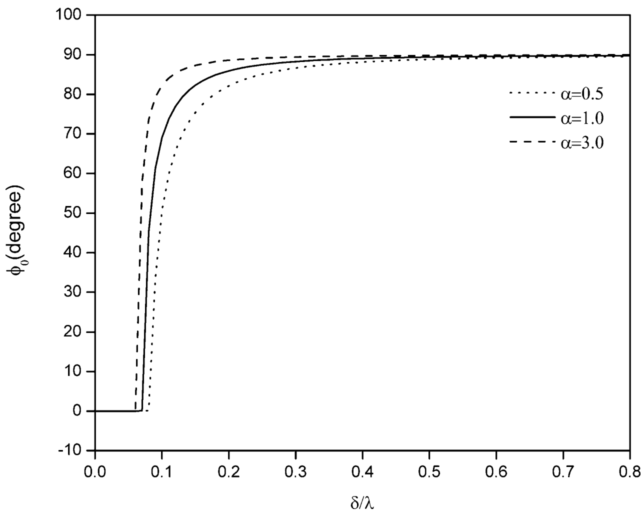

Figure 6. Twist angle ϕ_0 of lower substrate versus δ/λ for various values of α at saturation state. Material parameters used in the calculation as for figure 4.

$$
\begin{aligned}
l &= \lim_{\theta_0\to 0}\int_0^{\theta_0} N(0)\,\mathrm{d}\theta \\
&= \frac{l}{\pi}\int_0^{\frac{\pi}{2}} \frac{\cos\beta\,\mathrm{d}\beta}{\begin{aligned}&\{-u_s^2(1-\sin^2\beta)+ \\ &\alpha^2(rp-q+F/A_1)^2\frac{k_{11}(2k_{22}-k_{33})}{4k_{22}^2}\sin^2 2\phi_0(1-\sin^2\beta) \\ &+\alpha^2[rp-(r-1)q-F/A_1+(rp-q+F/A_1)\cos^2\phi_0]^2\}^{\frac{1}{2}}\end{aligned}}
\end{aligned} \qquad (55)
$$

where u_s is the reduced saturation voltage. Defining two parameters as

$$\kappa = \frac{k_{11}(2k_{22}-k_{33})}{4k_{22}^2} \qquad (56)$$

$$u_s' = \left[u_s^2-\alpha^2(rp-q+F/A_1)^2\kappa\sin^2 2\phi_0\right]^{\frac{1}{2}} \qquad (57)$$

and performing the integration of equation (55), we obtain

$$l = \frac{l}{\pi}\frac{1}{u_s'}\sinh^{-1}\frac{u_s'}{\left\{\begin{aligned}&\alpha^2[rp-(r-1)q- \\ &F/A+{}_1(rp-q+F/A_1)\cos^2\phi_0]^2-u_s'\end{aligned}\right\}^{\frac{1}{2}}}$$

or

$$u_s' = \left\{\begin{aligned}&\alpha^2[rp-(r-1)q-F/A_1+ \\ &(rp-q+F/A_1)\cos^2\phi_0]^2-u_s^2\end{aligned}\right\}^{\frac{1}{2}}\sinh(\pi u_s'). \qquad (58)$$

If $\phi_0\approx\frac{\pi}{2}$, equation (57) may be approximated as $u_s \approx u'_s$ and equation (58) may be approximated as

$$u_s = \left\{\alpha^2[rp-(r-1)q-F/A_1]^2-u_s^2\right\}^{\frac{1}{2}}\sinh(\pi u_s). \qquad (59)$$

These calculated results of reduced saturation voltage versus δ/λ with different α are shown in figure 7.

From figures 6 and 7, we see that ϕ_0 equals zero within $\delta/\lambda \leqslant 0.1$, then increases sharply, almost equal to 90° within $\delta/\lambda \geqslant 0.2$. Meanwhile u_s rises steadily within $\delta/\lambda \geqslant 0.2$. So we can conclude that appropriate values of λ and δ should be chosen in order to obtain larger values of ϕ_0 and smaller u_s. It may be noted that the shape of the curves of $\phi_0 \sim \delta/\lambda$ and $u_s \sim \delta/\lambda$ for a given λ depends on the values of r, $\bar{k}$ and α.

5. Discussion

We have studied two topics, the equivalent anchoring energy of a grating surface, and the VCT effect. In this section we shall discuss two problems:

5.1. *Equivalent anchoring energy of a grating surface*

The equivalent anchoring energy formulae (12) and (14) are based on the argument that the grating surface is a smooth curved surface with a continuous derivative, and is simplified into a cosinoidal surface. Any defect (such as a disclination) in the NLC near surface and corresponding free energy are ignored. Moreover, we have taken the approximation that θ and ϕ are functions of z only and not related to x. Our approximation appears be suitable only for $\delta \ll l$.

In our derivation of the formulae (12) and (14), the Berreman approximation is adopted. The HAN cell with a grating surface can be solved by the analytical

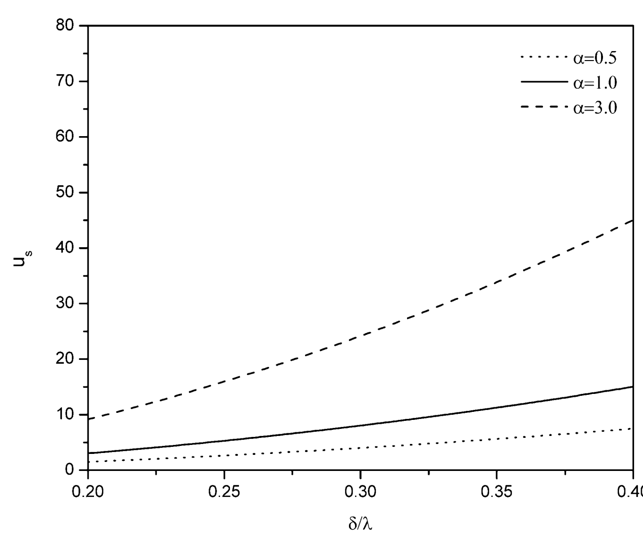

Figure 7. Variation of reduced saturation voltage versus δ/λ for various values of α. Material parameters as for figure 4.

method, provided that a variable transformation from z to $z'=l\frac{z-\delta\cos(qx)}{l-\delta\cos(qx)}$ is made, and the Berreman approximation can be explained. We will report this result elsewhere.

5.2. *Bistable state for grating surface*

Except VCT effect the bistable state may be appeared in HAN cell with grating surface. The equations (32) and (33) and corresponding boundary conditions equations (34) and (35) have the solution $\theta\equiv0$, a trivial solution in the mathematics, while the solutions of equations (42) and (43) are non-trivial solutions. In this paper, we only discuss the non-trivial solution. As in [19–21], the bistable state can be obtained if trivial and non-trivial solutions are considered together. We will report the bistable state in a later paper.

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