Influences of surface and flexoelectric polarization on the effective anchoring energy in nematic liquid crystal*

Guan Rong-Hua(关荣华)[a)†], Ye Wen-Jiang(叶文江)[b)‡], and Xing Hong-Yu(邢红玉)[b)]

[a)] School of Sciences, North China Electric Power University, Baoding 071003, China
[b)] School of Sciences, Hebei University of Technology, Tianjin 300401, China

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The physical effects on surface and flexoelectric polarization in a weak anchoring nematic liquid crystal cell are investigated systematically. We derive the analytic expressions of two effective anchoring energies for lower and upper substrates respectively as well as their effective anchoring strengths and corresponding tilt angles of effective easy direction. All of these quantities are relevant to the magnitudes of both two polarizations and the applied voltage U. Based on these expressions, the variations of effective anchoring strength and the tilt angle with the applied voltage are calculated for the fixed values of two polarizations. For an original weak anchoring hybrid aligned nematic cell, it may be equivalent to a planar cell for a small value of U and has a threshold voltage. The variation of reduced threshold voltage with reduced surface polarization strength is also calculated. The role of surface polarization is important without the adsorptive ions considered.

Keywords: surface and flexoelectric polarization, effective anchoring energy, easy direction, hybrid aligned nematic, threshold voltage

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1. Introduction

The anchoring phenomenon between liquid crystal (LC) and solid is usually described by the anchoring energy,[1] which can be seen as an anisotropic part of the interface energy. The expression of anchoring energy and its physical effects in the LC cell have been an important content of the LC surface physics.[2]

Physical reasons for the anchoring phenomenon and its microscopic mechanism are important subjects.[3] Recently, Yang *et al.*[4] have proposed that interface energy should be seen as the total sum of potentials between molecules of LC and the substrate surface. They gave out an expression of the anchoring energy, which turns into an RP formula in the one-dimensional (1D) case. However, the anchoring energy may originate from other physical reasons, such as adsorptive ions, surface polarization $\boldsymbol{P}_{\rm s}$ and flexoelectric polarization $\boldsymbol{P}_{\rm f}$, which induce the effective ahchoring energy on the substrate surface. The problem of effective anchoring energy induced by surface polarization or flexoelectric polarization has aroused the interest of many investigators.[5–14] Although adsorption ion exists inevitably in the real LC cell, the density of adsorptive ions is strongly dependent on the clean technology and cleaning time for the substrate. For a long cleaning time the density of adsorptive ions can be ignored. Hence, it is necessary to study these effects on the nematic liquid crystal (NLC) cell when the density of adsorptive ions is ignored.

In this paper, we investigate the physical effects of surface and flexoelectric polarization on the weak anchoring NLC cell for the case of ignoring the density of adsorptive ions, and put emphasis on the contributions of these two polarizations to the effective anchoring energy. Flexoelectric polarization $\boldsymbol{P}_{\rm f}$ can be expressed as[15]

$$\boldsymbol{P}_{\rm f} = e_{11}\boldsymbol{n}(\nabla\cdot\boldsymbol{n}) + e_{33}(\nabla\times\boldsymbol{n})\times\boldsymbol{n}, \tag{1}$$

where e_{11} and e_{33} are splay and bend flexoelectric coefficients, respectively, and $\boldsymbol{n}$ is the director of LC. Surface polarization $\boldsymbol{P}_{\rm s}$ can be induced by many reasons,[16] in which the order-electric polarization can be expressed as[17]

$$\boldsymbol{P}_{\rm s} = r_1(\boldsymbol{n}\cdot\operatorname{grad}S)\boldsymbol{n} + r_2\operatorname{grad}S. \tag{2}$$

where r_1 and r_2 are the order-electric coefficients, and S is the surface order parameter.

Based on the Frank elastic theory and Eqs. (1) and (2), the expression of the Gibbs free energy G for this NLC cell can be deduced. It consists of elastic, dielectric, polarization free energy, and anchoring energy. By calculating the variation of the Gibbs free energy G under a given voltage U using the method indicated in Ref. [18], we obtain the differential equation and the boundary conditions of the director. Then, the mathematical method to solve this equation with boundary conditions is given. Furthermore, we obtain the expressions

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†E-mail: ronghua_guan@163.com

‡Corresponding author. E-mail: wenjiang_ye@hebut.edu.cn

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of effective anchoring energy g_{s1eff} and g_{s2eff} for the lower and upper substrate respectively. We find that the anchoring strength and easy direction of effective anchoring energy vary with the applied voltage U no matter what the original anchoring is. For an original weak anchoring hybrid aligned nematic (HAN) cell, it may be equivalent to a planar cell for small values of U and has a threshold voltage.

2. Fundamental equations and their solution

We consider a weak anchoring NLC cell with two substrates perpendicular to the z-axis. An external voltage $U$is applied to the cell. Assuming that the director of LC is limited in the xoz-plane, the tilt angle θ of the director is only a function of z. The anchoring energy densities of the lower substrate (placed at $z=0$) and upper substrate (placed at $z=l$) are $g_{s1}=A_1\sin^2(\theta_0-\Theta_1)/2$ and $g_{s2}=A_2\sin^2(\theta_l-\Theta_2)/2$, where A_1 and A_2 are the anchoring strengths, θ_0 and θ_l are the tilt angles of the director, and Θ_1 and Θ_2 are the tilt angles of the easy direction $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ at the lower and upper substrate, respectively.

Suppose that the surface polarizations are $\boldsymbol{P}_{s1}$ and $\boldsymbol{P}_{s2}$ for the lower and the upper substrate, and they arise in very thin surface layers with thickness values δ_1 and δ_2 ($\delta_1, \delta_2 \ll l$) respectively, i.e., they satisfy the following conditions: $\boldsymbol{P}_{s1}=0$ for $z\geq\delta_1$ and $\boldsymbol{P}_{s2}=0$ for $z\leq l-\delta_2$. The total polarization is $\boldsymbol{P}=\boldsymbol{P}_f+\boldsymbol{P}_{s1}+\boldsymbol{P}_{s2}$. The dielectric displacement $\boldsymbol{D}$ should be $\boldsymbol{D}=\varepsilon_\perp\boldsymbol{E}+\Delta\varepsilon(\boldsymbol{n}\cdot\boldsymbol{E})\boldsymbol{n}+\boldsymbol{P}$, where $\Delta\varepsilon=\varepsilon_{//}-\varepsilon_\perp$ is the anisotropy of the dielectric constant, $\varepsilon_{//}$ and $\varepsilon_\perp$ are the dielectric constants parallel and perpendicular to the director respectively. Because $\nabla\cdot\boldsymbol{D}=0$, the z component of the dielectric displacement, $D_z=(\varepsilon_\perp+\Delta\varepsilon\sin^2\theta)E_z+P_z$, is a constant for $0\leq z\leq l$. The applied voltage can be expressed as

$$U=\int_0^l E_z\mathrm{d}z=D_z\int_0^l\frac{\mathrm{d}z}{g(\theta)}-\int_0^l\frac{P_z}{g(\theta)}\mathrm{d}z, \tag{3}$$

where $g(\theta)=\varepsilon_\perp+\Delta\varepsilon\sin^2\theta$.

The total Gibbs free energy per unit area of substrate can be expressed as

$$G=\int_0^l\left(f_{elas}+f_{diel}+f_{polar}\right)\mathrm{d}z+g_{s1}+g_{s2}, \tag{4}$$

where f_{elas}, f_{diel}, and f_{polar} denote the free energy density of elastic, dielectric, and polarization respectively, and can be expressed as $f_{elas}=f(\theta)\theta'^2/2$, $f_{diel}=-g(\theta)E_z^2/2$, $f_{polar}=-P_zE_z$, $\theta'=\mathrm{d}\theta/\mathrm{d}z$, $f(\theta)=k_{11}\cos^2\theta+k_{33}\sin^2\theta$, k_{11} and k_{33} are the splay and bend elastic constants, respectively. Substituting the expressions of g_{s1} and g_{s2} into Eq. (4), the expression of Gibbs free energy becomes

$$\begin{aligned}G=&\frac{1}{2}\int_0^l f_{eff}(\theta)\theta'^2\mathrm{d}z-\frac{1}{2}\frac{U_{eff}^2}{\int_0^l\frac{\mathrm{d}z}{g(\theta)}}+\frac{1}{2}\int_0^{\delta_1}\frac{P_{s1z}^2}{g(\theta)}\mathrm{d}z\\&+\frac{1}{2}\int_{l-\delta_2}^l\frac{P_{s2z}^2}{g(\theta)}\mathrm{d}z+\frac{e_1+e_3}{2}\int_0^{\delta_1}\frac{\sin2\theta\cdot\theta'P_{s1z}}{g(\theta)}\mathrm{d}z\\&+\frac{e_{11}+e_{33}}{2}\int_{l-\delta_2}^l\frac{\sin2\theta\cdot\theta'P_{s2z}}{g(\theta)}\mathrm{d}z+\frac{1}{2}A_1\sin^2(\theta_0-\Theta_1)\\&+\frac{1}{2}A_2\sin^2(\theta_l-\Theta_2),\end{aligned} \tag{5}$$

where

$$f_{eff}(\theta)=f(\theta)+\frac{(e_{11}+e_{33})^2}{4}\frac{\sin^2(2\theta)}{\varepsilon_\perp+\Delta\varepsilon\sin^2\theta}.$$

The differential equation and the boundary conditions of $\theta(z)$ can be derived by calculating the variation of G for given voltage U using the method explained in Ref. [18]. Suppose that $\bar{\theta}(z)$ is the solution which makes G minimal and then $\theta(z)$ can be expressed as

$$\theta(z)=\bar{\theta}(z)+\eta\xi(z), \tag{6}$$

where $\xi(z)$ is an arbitrary function of z, and η is a common variable. Substituting Eq. (6) into Eq. (5), the resulting G becomes a common function of η. According to $\partial G/\partial\eta|_{\eta=0}=0$, we obtain the equation and the boundary conditions of $\theta(z)$ as follows:

$$\frac{1}{2}\frac{\partial f_{eff}(\theta)}{\partial\theta}\theta'^2-\frac{\partial}{\partial z}\left[f_{eff}(\theta)\theta'\right]-\frac{1}{2}D_z^2\frac{\Delta\varepsilon\sin2\theta}{[g(\theta)]^2}=0, \tag{7}$$

$$\begin{aligned}&f_{eff}(\theta_l)\theta_l'-\frac{e_1+e_3}{2}D_z\frac{\sin2\theta_l}{g(\theta_l)}+\frac{e_{11}+e_{33}}{2}\frac{P_{s2z}\sin2\theta_l}{g(\theta_l)}\\&\quad+\frac{1}{2}A_2\sin2(\theta_l-\Theta_2)=0,\end{aligned} \tag{8}$$

$$\begin{aligned}&f_{eff}(\theta_0)\theta_0'-\frac{e_1+e_3}{2}D_z\frac{\sin2\theta_0}{g(\theta_0)}+\frac{e_{11}+e_{33}}{2}\frac{P_{s1z}\sin2\theta_0}{g(\theta_0)}\\&\quad-\frac{1}{2}A_1\sin2(\theta_0-\Theta_1)=0,\end{aligned} \tag{9}$$

where $\theta_0'=(\mathrm{d}\theta/\mathrm{d}z)_{\theta=\theta_0}$, $\theta_l'=(\mathrm{d}\theta/\mathrm{d}z)_{\theta=\theta_l}$, and we neglect all terms proportional to δ_1 or δ_2 by considering that the values of P_f and P_s have the same order of magnitude and $\delta_1\ll l$, $\delta_2\ll l$. The mathematical progress is presented in Appendix A. Equations (7)–(9) are the fundamental equations of NLC cell.

Now we discuss the solution of Eq. (7) with boundary conditions Eqs. (8) and (9). From Eq. (7) if $\theta'\neq0$ we obtain[1)]

$$\frac{\mathrm{d}}{\mathrm{d}z}\left[f_{eff}(\theta)\theta'^2-\frac{D_z^2}{g(\theta)}\right]=0, \tag{10}$$

then

$$f_{eff}(\theta)\theta'^2-\frac{D_z^2}{g(\theta)}=C, \tag{11}$$

where C is a constant, which can be expressed as $C=f_{eff}(\theta_0)\theta_0'^2-D_z^2/g(\theta_0)$ or $C=f_{eff}(\theta_l)\theta_l'^2-D_z^2/g(\theta_l)$. If $\theta'=$

[1)] If $\Theta_1, \Theta_2=0, \pi/2$, then both $\theta\equiv0$ and $\theta\equiv\pi/2$ may be the solutions also. For these cases, $\theta'=0$.

0 at $z = d$ $(0 < d < l)$ and $\theta_d = \theta_{\max}$, then C can be expressed as $C = -D_z^2/g(\theta_{\max})$. If we put

$$M(\theta) = \sqrt{\frac{f_{\text{eff}}(\theta)\, g(\theta)}{\dfrac{C g(\theta)}{D_z^2} + 1}}, \tag{12}$$

then

$$\mathrm{d}z = \pm \frac{M(\theta)}{D_z}\mathrm{d}\theta, \tag{13}$$

where "±" can be determined according to the actual case. Then θ can be obtained by integrating Eq. (13).

The concrete expression of $M(\theta)$ is determined by the expression of constant C. There are four different cases as follows:

i) $\theta' > 0$ for $0 \le z \le l$, the value of θ_l is largest and function θ can be expressed as

$$z = \int_{\theta_0}^{\theta} \frac{M(\theta)}{D_z}\mathrm{d}\theta;$$

ii) $\theta' < 0$ for $0 \le z \le l$, the value of θ_0 is largest and function θ can be expressed as

$$z = \int_{\theta}^{\theta_0} \frac{M(\theta)}{D_z}\mathrm{d}\theta;$$

iii) $\theta' > 0$ for $0 \le z < d$, $\theta' < 0$ for $d < z \le l$, and $\theta' = 0$ at $z = d$, the value of θ at $z = d$ is the maximum, denoted by $\theta_{\max}$. $M(\theta)$ can be expressed as

$$M(\theta) = \sqrt{\frac{f_{\text{eff}}(\theta)\, g(\theta)\, g(\theta_{\max})}{\Delta\varepsilon\left(\sin^2\theta_{\max} - \sin^2\theta\right)}}, \tag{14}$$

and function θ can be expressed as

$$z = \int_{\theta_0}^{\theta} \frac{M(\theta)}{D_z}\mathrm{d}\theta$$

for $0 \le z < d$, and

$$z = l - \int_{\theta_l}^{\theta} \frac{M(\theta)}{D_z}\mathrm{d}\theta;$$

for $d < z \le l$;

iv) $\theta' < 0$ for $0 \le z < d$, $\theta' > 0$ for $d < z \le l$, and $\theta' = 0$ at $z = d$, the value of θ at $z = d$ is the minimum, denoted by $\theta_{\min}$. The expression of $M(\theta)$ is the same as Eq. (14) and function θ can be expressed as

$$z = \int_{\theta}^{\theta_0} \frac{M(\theta)}{D_z}\mathrm{d}\theta$$

for $0 \le z < d$, and

$$z = l - \int_{\theta}^{\theta_l} \frac{M(\theta)}{D_z}\mathrm{d}\theta$$

for $d < z \le l$.

3. Effective anchoring energy and their properties

Equations (8) and (9) can be seen as the balance equations of "forces" acting on the director at the interfaces. From the expressions of these "forces", one can deduce the expressions of corresponding "potential". In this way, we may obtain the expressions of effective anchoring energy.

Equations (8) and (9) may be re-expressed as

$$\begin{aligned} -f_{\text{eff}}(\theta_l)\,\theta_l' &= \frac{1}{2}A_2 \sin 2(\theta_l - \Theta_2) - \frac{e_{11}+e_{33}}{2}\frac{D_z}{g(\theta_l)}\sin 2\theta_l \\ &\quad + \frac{e_{11}+e_{33}}{2}\frac{P_{\text{s}2z}}{g(\theta_l)}\sin 2\theta_l, \end{aligned} \tag{15}$$

$$\begin{aligned} f_{\text{eff}}(\theta_0)\,\theta_0' &= \frac{1}{2}A_1 \sin 2(\theta_0 - \Theta_1) + \frac{e_{11}+e_{33}}{2}\frac{D_z}{g(\theta_0)}\sin 2\theta_0 \\ &\quad - \frac{e_{11}+e_{33}}{2}\frac{P_{\text{s}1z}}{g(\theta_0)}\sin 2\theta_0. \end{aligned} \tag{16}$$

By comparing Eqs. (15) and (16) with the boundary conditions of the same NLC cell without these two polarizations $\boldsymbol{P}_{\text{s}}$ and $\boldsymbol{P}_{\text{f}}$, the effective anchoring energy g_{s2eff} and g_{s1eff} satisfy the following equations respectively

$$\begin{aligned} \frac{\partial}{\partial\theta_l} g_{\text{s2eff}}(\theta_l) &= \frac{1}{2}A_2 \sin 2(\theta_l - \Theta_2) - \frac{e_{11}+e_{33}}{2}\frac{D_z}{g(\theta_l)}\sin 2\theta_l \\ &\quad + \frac{e_{11}+e_{33}}{2}\frac{P_{\text{s}2z}}{g(\theta_l)}\sin 2\theta_l, \end{aligned} \tag{17}$$

$$\begin{aligned} \frac{\partial}{\partial\theta_0} g_{\text{s1eff}}(\theta_0) &= \frac{1}{2}A_1 \sin 2(\theta_0 - \Theta_1) + \frac{e_{11}+e_{33}}{2}\frac{D_z}{g(\theta_0)}\sin 2\theta_0 \\ &\quad + \frac{e_{11}+e_{33}}{2}\frac{P_{\text{s}1z}}{g(\theta_0)}\sin 2\theta_0. \end{aligned} \tag{18}$$

Therefore, g_{s2eff} and g_{s1eff} can be obtained by means of the indefinite integral, expressed as

$$\begin{aligned} g_{\text{s2eff}} &= \frac{1}{2}A_2 \sin^2(\theta_l - \Theta_2) - \int \frac{(e_{11}+e_{33})D_z \sin 2\theta_l}{2g(\theta_l)}\mathrm{d}\theta_l \\ &\quad + \frac{(e_{11}+e_{33})P_{\text{s}2}^0}{2\Delta\varepsilon}\left[r\sin^2\theta_l + \left(1 - \frac{\varepsilon_\perp r}{\Delta\varepsilon}\right)\ln g(\theta_l)\right], \end{aligned} \tag{19}$$

$$\begin{aligned} g_{\text{s1eff}} &= \frac{1}{2}A_1 \sin^2(\theta_0 - \Theta_1) + \int \frac{(e_{11}+e_{33})D_z \sin\theta_0}{2g(\theta_0)}\mathrm{d}\theta_0 \\ &\quad - \frac{(e_{11}+e_{33})P_{\text{s}1}^0}{2\Delta\varepsilon}\left[r\sin^2\theta_0 + \left(1 - \frac{\varepsilon_\perp r}{\Delta\varepsilon}\right)\ln g(\theta_0)\right], \end{aligned} \tag{20}$$

where $r = r_1/r_2$,

$$P_{\text{s}1}^0 = r_2 \left.\frac{\mathrm{d}S}{\mathrm{d}z}\right|_{z=0},$$

and

$$P_{\text{s}2}^0 = r_2 \left.\frac{\mathrm{d}S}{\mathrm{d}z}\right|_{z=l}.$$

Note that D_z is a function of θ_0 and θ_l, and its expression is complex (see Appendix B), so that the corresponding terms of

expressions (19) and (20) are expressed as an indefinite integral form for the time being.

Now we discuss the effective easy direction $e_{1\mathrm{eff}}$ and $e_{2\mathrm{eff}}$ as well as the effective anchoring strength $A_{1\mathrm{eff}}$ and $A_{2\mathrm{eff}}$. We use ω_1 and ω_2 to represent the tilt angles of effective easy direction $e_{1\mathrm{eff}}$ and $e_{2\mathrm{eff}}$ respectively. According to Ref. [3], they can be determined by the following equations:

$$\left.\frac{\partial g_{\mathrm{s1eff}}}{\partial\theta_0}\right|_{\theta_0=\omega_1}=0,\quad \left.\frac{\partial^2 g_{\mathrm{s1eff}}}{\partial\theta_0^2}\right|_{\theta_0=\omega_1}>0; \tag{21}$$

$$\left.\frac{\partial g_{\mathrm{s2eff}}}{\partial\theta_l}\right|_{\theta_l=\omega_2}=0,\quad \left.\frac{\partial^2 g_{\mathrm{s2eff}}}{\partial\theta_l^2}\right|_{\theta_l=\omega_2}>0. \tag{22}$$

According to Ref. [19], for a small deviation of the director $\boldsymbol{n}$ from easy direction $\boldsymbol{e}$, the anchoring energy may be expressed as $g_{\mathrm{s}}=A\sin^2(\theta-\omega)/2$, where θ and ω are the tilt angles of $\boldsymbol{n}$ and $\boldsymbol{e}$ respectively, A is the anchoring energy strength at the substrate surface. Generally speaking, the anchoring energy may be expressed as $g_{\mathrm{s}}=c_0+c_1\sin^2(\theta-\omega)+c_2\sin^4(\theta-\omega)+\cdots$, where c_0, c_1, c_2, ... are constants. If the value of $\theta-\omega$ is small, the anchoring strength A is equal to $2c_1$.

Consider g_{s1eff} first. θ and ω in the expression of $g_{\mathrm{s}}=A\sin^2(\theta-\omega)/2$ are written as θ_0 and ω_1 at present. In this case, by making a variable transformation from θ_0 to t, $t=\sin(\theta_0-\omega_1)$, g_{s1eff} is a function of t. It can be expanded in Taylor's series at $t=0$ (i.e. $\theta_0=\omega_1$) as

$$g_{\mathrm{s1eff}}=g_{\mathrm{s1eff}}|_{t=0}+\left.\frac{\partial g_{\mathrm{s1eff}}}{\partial t}\right|_{t=0}t+\frac{1}{2!}\left.\frac{\partial^2 g_{\mathrm{s1eff}}}{\partial t^2}\right|_{t=0}t^2+\cdots. \tag{23}$$

Because

$$\left.\frac{\partial g_{\mathrm{s1eff}}}{\partial t}\right|_{t=0}=\left.\frac{\partial g_{\mathrm{s1eff}}}{\partial\theta_0}\right|_{\theta_0=\omega_1}=0$$

and

$$\left.\frac{\partial^2 g_{\mathrm{s1eff}}}{\partial t^2}\right|_{t=0}=\left.\frac{\partial^2 g_{\mathrm{s1eff}}}{\partial\theta_0^2}\right|_{\theta_0=\omega_1},$$

the effective anchoring strength of the lower substrate can be expressed as

$$A_{1\mathrm{eff}}=\left.\frac{\partial^2 g_{\mathrm{s1eff}}}{\partial\theta_0^2}\right|_{\theta_0=\omega_1}, \tag{24}$$

meanwhile the second equation in Eq. (21) is equivalent to $A_{1\mathrm{eff}}>0$.

Similarly, for g_{s2eff}, ω_2 and $A_{2\mathrm{eff}}$ may be solved from the following two equations:

$$\left.\frac{\partial g_{\mathrm{s2eff}}}{\partial\theta_l}\right|_{\theta_l=\omega_2}=0, \tag{25}$$

$$A_{2\mathrm{eff}}=\left.\frac{\partial^2 g_{\mathrm{s2eff}}}{\partial\theta_l^2}\right|_{\theta_l=\omega_2}, \tag{26}$$

and the second equation in Eq. (22) is equivalent to $A_{2\mathrm{eff}}>0$.

By using the method stated above, we may obtain the effective anchoring strength and easy direction. For g_{s1eff}, there are two equations to determine ω_1 and $A_{1\mathrm{eff}}$, i.e.,

$$\begin{aligned}&\left.\frac{\partial g_{\mathrm{s1eff}}}{\partial\theta_0}\right|_{\theta_0=\omega_1}\\&=\frac{1}{2}A_1\sin 2(\omega_1-\Theta_1)-\frac{e_{11}+e_{33}}{2\Delta\varepsilon}P_{\mathrm{s1}}^0 r\sin 2\omega_1+\frac{e_{11}+e_{33}}{2g(\omega_1)}\\&\times\left(D_z-P_{\mathrm{s1}}^0+\frac{\varepsilon_\perp}{\Delta\varepsilon}P_{\mathrm{s1}}^0 r\right)\sin 2\omega_1=0,\end{aligned} \tag{27}$$

$$\begin{aligned}&A_{1\mathrm{eff}}\\&=\left.\frac{\partial^2 g_{\mathrm{s1eff}}}{\partial\theta_0^2}\right|_{\theta_0=\omega_1}\\&=A_1\cos 2(\omega_1-\Theta_1)-\frac{e_{11}+e_{33}}{\Delta\varepsilon}P_{\mathrm{s1}}^0 r\cos 2\omega_1\\&+\frac{e_{11}+e_{33}}{g(\omega_1)}\left[\cos 2\omega_1-\frac{\Delta\varepsilon}{2g(\omega_1)}\sin^2 2\omega_1\right]\\&\times\left(D_z-P_{\mathrm{s1}}^0+\frac{\varepsilon_\perp}{\Delta\varepsilon}P_{\mathrm{s1}}^0 r\right)+\frac{e_{11}+e_{33}}{2g(\omega_1)}\sin 2\omega_1\left.\frac{\partial D_z}{\partial\theta_0}\right|_{\theta_0=\omega_1}\\&>0.\end{aligned} \tag{28}$$

Their solutions are relevant to Θ_1. As an example, if $\Theta_1=0$, equation (27) has three solutions: $\omega_1=0$, $\pi/2$, and $\sin^{-1}R_1$, where

$$R_1^2=\frac{(e_{11}+e_{33})(P_{\mathrm{s1}}^0-D_z)-A_1\varepsilon_\perp}{A_1\Delta\varepsilon-(e_{11}+e_{33})P_{\mathrm{s1}}^0 r}, \tag{29}$$

if $0\le R_1^2\le 1$. For each value of ω_1, the corresponding effective anchoring strength $A_{1\mathrm{eff}}$ may be calculated from Eq. (24). The results are shown in Table 1 and the mathematical process is explained in Appendix B. For the case $\Theta_1=\pi/2$, $A_{1\mathrm{eff}}$ and ω_1 can be obtained also (see Table 1).

Adopting the same method, we obtain the tilt angle ω_2 and the effective anchoring strength $A_{2\mathrm{eff}}$ for $g_{2\mathrm{eff}}$, see Table 2, where

$$R_2^2=\frac{e_{11}+e_{33}(D_z-P_{\mathrm{s2}}^0)-A_2\varepsilon_\perp}{A_2\Delta\varepsilon+(e_{11}+e_{33})P_{\mathrm{s2}}^0 r}. \tag{30}$$

4. Threshold voltage for weak HAN cell

We have explained the mathematical method to solve Eq. (7) under the boundary conditions Eqs. (8) and (9) in Section 2. Now, we consider an original weak anchoring HAN cell with $\Theta_1=0$ and $\Theta_2=\pi/2$. There are four cases discussed in Section 2. Case iii) and case iv) are more particular, and these two cases are similar. Thus, we consider case iii). In this case, $\theta_0'>0$ and $\theta_l'<0$, from Eqs. (8) and (9) we have

$$A_1-\frac{e_{11}+e_{33}}{g(\theta_0)}(P_{\mathrm{s1}z}-D_z)>0, \tag{31}$$

$$A_2-\frac{e_{11}+e_{33}}{g(\theta_l)}(P_{\mathrm{s2}z}-D_z)<0. \tag{32}$$

Table 1. Effective anchoring strengths and easy directions for g_{s1eff}.

Θ_1 \ A_{1eff} \ ω	0	$\pi/2$	$\sin^{-1}R_1$
0	$A_{1eff}=A_1-\frac{e_{11}+e_{33}}{\varepsilon_\perp}$ $\times\left(P_{s1}^0-D_z\right)$	$A_{1eff}=-A_1+\frac{e_{11}+e_{33}}{\varepsilon_\parallel}$ $\times\left[P_{s1}^0(1+r)-D_z\right]$	$A_{1eff}=\frac{\left[A_1-\frac{e_{11}+e_{33}}{\varepsilon_\perp}\left(D_z-P_{s1}^0\right)\right]\left[A_1-\frac{e_{11}+e_{33}}{\varepsilon_\parallel}\left[D_z-P_{s1}^0(1+r)\right]\right]}{\frac{e_{11}+e_{33}}{2}\left(\frac{1}{\varepsilon_\perp}-\frac{1}{\varepsilon_\parallel}\right)\left[D_z-P_{s1}^0+\frac{\varepsilon_\perp}{\Delta\varepsilon}P_{s1}^0 r\right]^2}$ $\times\left(D_z-P_{s1}^0+\frac{\varepsilon_\perp}{\Delta\varepsilon}P_{s1}^0 r+\Delta_1\right)$
$\pi/2$	$A_{1eff}=-A_1-\frac{e_{11}+e_{33}}{\varepsilon_\perp}$ $\times\left(P_{s1}^0-D_z\right)$	$A_{1eff}=A_1+\frac{e_{11}+e_{33}}{\varepsilon_\parallel}$ $\times\left[P_{s1}^0(1+r)-D_z\right]$	$A_{1eff}=\frac{\left[A_1-\frac{e_{11}+e_{33}}{\varepsilon_\perp}\left(D_z-P_{s1}^0\right)\right]\left[A_1-\frac{e_{11}+e_{33}}{\varepsilon_\parallel}\left[D_z-P_{s1}^0(1+r)\right]\right]}{\frac{e_{11}+e_{33}}{2}\left(\frac{1}{\varepsilon_\perp}-\frac{1}{\varepsilon_\parallel}\right)\left[D_z-P_{s1}^0+\frac{\varepsilon_\perp}{\Delta\varepsilon}P_{s1}^0 r\right]^2}$ $\times\left(D_z-\beta_1+\frac{\varepsilon_\perp}{\Delta\varepsilon}P_{s1}^0 r+\Delta_1\right)$

Table 2. Effective anchoring strengths and easy directions for g_{s2eff}.

Θ_1 \ A_{2eff} \ ω	0	$\pi/2$	$\sin^{-1}R_1$
0	$A_{2eff}=A_2-\frac{e_{11}+e_{33}}{\varepsilon_\perp}$ $\times\left(D_z-P_{s2}^0\right)$	$A_{2eff}=-A_2+\frac{e_{11}+e_{33}}{\varepsilon_\parallel}$ $\times\left[D_z-P_{s2}^0(1+r)\right]$	$A_{2eff}=\frac{\left[-A_2+\frac{e_{11}+e_{33}}{\varepsilon_\perp}\left(D_z-P_{s2}^0\right)\right]\left[A_2-\frac{e_{11}+e_{33}}{\varepsilon_\parallel}\left[D_z-P_{s2}^0(1+r)\right]\right]}{\frac{e_{11}+e_{33}}{2}\left(\frac{1}{\varepsilon_\perp}-\frac{1}{\varepsilon_\parallel}\right)\left[D_z-P_{s2}^0+\frac{\varepsilon_\perp}{\Delta\varepsilon}P_{s2}^0 r\right]^2}$ $\times\left(D_z-P_{s2}^0+\frac{\varepsilon_\perp}{\Delta\varepsilon}P_{s2}^0 r+\Delta_2\right)$
$\pi/2$	$A_{2eff}=-A_2-\frac{e_{11}+e_{33}}{\varepsilon_\perp}$ $\times\left(D_z-P_{s2}^0\right)$	$A_{2eff}=A_2+\frac{e_{11}+e_{33}}{\varepsilon_\parallel}$ $\times\left[D_z-P_{s2}^0(1+r)\right]$	$A_{2eff}=\frac{\left[A_2+\frac{e_{11}+e_{33}}{\varepsilon_\perp}\left(D_z-P_{s2}^0\right)\right]\left[-A_2-\frac{e_{11}+e_{33}}{\varepsilon_\parallel}\left[D_z-P_{s2}^0(1+r)\right]\right]}{\frac{e_{11}+e_{33}}{2}\left(\frac{1}{\varepsilon_\perp}-\frac{1}{\varepsilon_\parallel}\right)\left[D_z-P_{s2}^0+\frac{\varepsilon_\perp}{\Delta\varepsilon}P_{s2}^0 r\right]^2}$ $\times\left(D_z-P_{s2}^0+\frac{\varepsilon_\perp}{\Delta\varepsilon}P_{s2}^0 r+\Delta_2\right)$

If equations (31) and (32) hold for $0\le z\le l$, these two equations mean that the two effective anchoring strengths are

$$A_{1eff}=A_1-\frac{e_{11}+e_{33}}{\varepsilon_\perp}\left(P_{s1}^0-D_z\right)>0, \tag{33}$$

$$A_{2eff}=-A_2+\frac{e_{11}+e_{33}}{\varepsilon_\perp}\left(P_{s2}^0-D_z\right)>0, \tag{34}$$

and the tilt angles of the easy direction $\boldsymbol{e}_{1eff}$ and $\boldsymbol{e}_{2eff}$ of the effective anchoring are $\omega_1=0$ and $\omega_2=0$, as stated in Section 3 (see Tables 1 and 2). This is to say, the original HAN cell is equivalent to a planar cell in this situation.

Now we return to discuss the conditions Eqs. (33) and (34). Several quantities P_{s1}^0, P_{s2}^0, and D_z, are represented as

$$P_{s1}^0=r_2\left.\frac{\mathrm{d}S}{\mathrm{d}z}\right|_{z=0},\quad P_{s2}^0=r_2\left.\frac{\mathrm{d}S}{\mathrm{d}z}\right|_{z=l},$$

$$D_z=\frac{U+U_a}{\int_0^l\frac{\mathrm{d}z}{g(\theta)}},\quad U_a=\frac{e_{11}+e_{33}}{2\Delta\varepsilon}\ln\frac{g(\theta_l)}{g(\theta_0)}.$$

Equations (33) and (34) may be rewritten as

$$A_{1eff}=A_1+\frac{(e_{11}+e_{33})^2}{6\varepsilon_\perp}\frac{1}{S}\left.\frac{\mathrm{d}S}{\mathrm{d}z}\right|_{z=0}+\frac{e_{11}+e_{33}}{\varepsilon_\perp}\frac{U}{\int_0^l\frac{\mathrm{d}z}{g(\theta)}}+\frac{(e_{11}+e_{33})^2}{2\varepsilon_\perp\Delta\varepsilon}\frac{\ln g(\theta_l)-\ln g(\theta_0)}{\int_0^l\frac{\mathrm{d}z}{g(\theta)}}>0, \tag{35}$$

$$A_{2eff}=-A_2-\frac{(e_{11}+e_{33})^2}{6\varepsilon_\perp}\frac{1}{S}\left.\frac{\mathrm{d}S}{\mathrm{d}z}\right|_{z=l}-\frac{e_{11}+e_{33}}{\varepsilon_\perp}\frac{U}{\int_0^l\frac{\mathrm{d}z}{g(\theta)}}-\frac{(e_{11}+e_{33})^2}{2\varepsilon_\perp\Delta\varepsilon}\frac{\ln g(\theta_l)-\ln g(\theta_0)}{\int_0^l\frac{\mathrm{d}z}{g(\theta)}}>0. \tag{36}$$

According to Ref. [6], $r_2=-(e_{11}+e_{33})/6S$, and $r=r_1/r_2=-3$. From Eq. (36) we see that the case $[\mathrm{d}S/\mathrm{d}z]_{z=l}<0$ is favourable, which means that it should be $P_{s2}^0>0$ for $e_{11}+e_{33}>0$, and $P_{s2}^0<0$ for $e_{11}+e_{33}<0$. If these equations hold for a small value of U (up to $U=0$), then there is a threshold voltage for this cell.

Substituting Eq. (14) into Eqs. (8) and (9), the boundary conditions can be re-expressed as

$$\frac{1}{2}\left(A_1-\frac{e_{11}+e_{33}}{g(\theta_0)}P_{s1z}\right)\sin 2\theta_0=D_z\left\{\frac{f_{eff}(\theta_0)}{M(\theta_0)}-\frac{e_{11}+e_{33}}{2}\frac{\sin 2\theta_0}{g(\theta_0)}\right\}, \tag{37}$$

$$\frac{1}{2}\left(\frac{e_{11}+e_{33}}{g(\theta_l)}P_{s2z}-A_2\right)\sin 2\theta_l = D_z\left\{\frac{f_{\rm eff}(\theta_l)}{M(\theta_l)}+\frac{e_{11}+e_{33}}{2}\frac{\sin 2\theta_l}{g(\theta_l)}\right\}. \quad (38)$$

In order to calculate the threshold voltage, we take a transformation $\sin\alpha = \sin\theta/\sin\theta_{\max}$. The threshold voltage $U_{\rm th}$ may be obtained from Eqs. (14), (37), and (38) by using the condition $\theta_{\max}\to 0$. Introducing some reduced parameters: reduced voltage $u = U/\pi\sqrt{k_{11}/\Delta\varepsilon}$, reduced threshold voltage $u_{\rm th} = U_{\rm th}/\pi\sqrt{k_{11}/\Delta\varepsilon}$, reduced anchoring strength $a_1 = A_1 l/2k_{11}$, $a_2 = A_2 l/2k_{11}$, reduced flexoelectric coefficient $e = (e_{11}+e_{33})/\sqrt{k_{11}\varepsilon_\perp}$ and reduced strength of surface polarization $p_1 = P_{s1}^0 l/2\sqrt{k_{11}\varepsilon_\perp}$ and $p_2 = P_{s2}^0 l/2\sqrt{k_{11}\varepsilon_\perp}$, the reduced threshold voltage can be expressed as

$$\tan(\pi u_{\rm th}) = \frac{2(a_1-ep_1-a_2+ep_2)\pi u_{\rm th}}{\left(1-\frac{\varepsilon_\perp}{\Delta\varepsilon}e^2\right)(\pi u_{\rm th})^2 - 2e\sqrt{\frac{\varepsilon_\perp}{\Delta\varepsilon}}(a_1-ep_1+a_2-ep_2)\pi u_{\rm th}+4(a_1-ep_1)(a_2-ep_2)}. \quad (39)$$

According to Eq. (39), we calculate the dependences of the reduced threshold voltage $u_{\rm th}$ on the surface polarization strength p_1 under different parameters. The results are shown in Fig. 1. The material parameters of LC are $k_{11} = 13.2$ pN, $k_{33} = 18.3$ pN, and $\Delta\varepsilon = 4.8$. The thickness of the NLC cell is $l = 10$ μm.

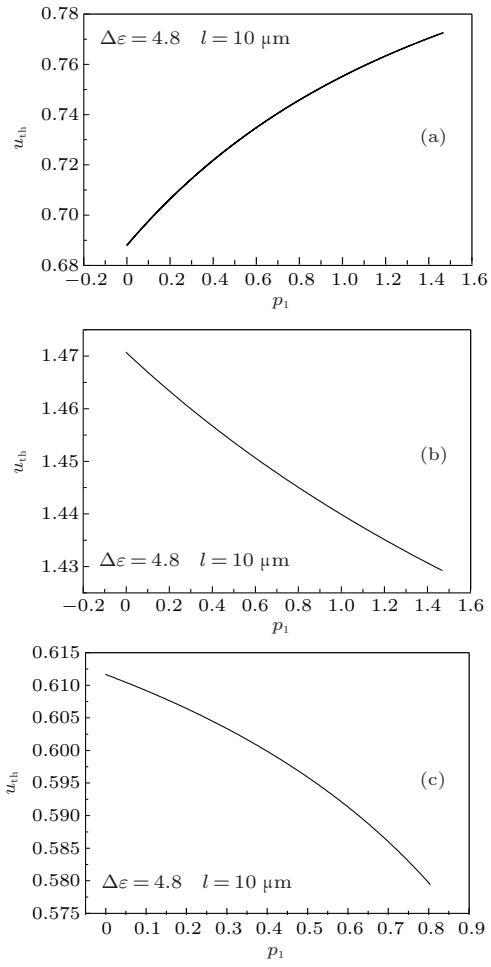


Fig. 1. Variations of the reduced threshold voltage $u_{\rm th}$ with the reduced strength of surface polarization p_1 under different parameters: (a) $e_{11}+e_{33} = -4.5\times10^{-11}$ C/m, $P_{s2}^0 = -2.0$ μC/m^2, $A_1 = 1.0\times10^{-5}$ J/m^2, $A_2 = 1.0\times10^{-6}$ J/m^2; (b) $e_{11}+e_{33} = -4.5\times10^{-11}$ C/m, $P_{s2}^0 = 0.29$ μC/m^2, $A_1 = 4.0\times10^{-5}$ J/m^2, $A_2 = 1.0\times10^{-5}$ J/m^2; (c) $e_1+e_3 = 4.5\times10^{-11}$ C/m, $P_{s2}^0 = 8.0$ μC/m^2, $A_1 = 4.0\times10^{-6}$ J/m^2, $A_2 = 1.0\times10^{-6}$ J/m^2.

5. Effective anchoring strength and corresponding easy direction for weak HAN cell

Now, we continue the discussion of the original weak anchoring HAN cell. We calculate the values of $A_{1\rm eff}$ and $A_{2\rm eff}$ as well as ω_1 and ω_2 with different values of U by using Eqs. (7)–(9). About the measurement of the flexoelectric coefficient, different research groups have been done using different methods.[20–24] Even for the same kind of LC materials, the value of flexoelectric coefficient is not the same. However, Castles *et al.*[25,26] have proved that the flexoelectric coefficient in NLC has a clear fundamental limit to the conventional order of magnitude of 10^{-11} C/m from conservation of energy considerations. On the selection of surface polarization, we adopt the measurement value given in Ref. [27]. In order to put emphasis on the effects of two polarizations, especially the surface polarization, we adopt three sets of parameters in calculation: (i) $e_{11}+e_{33} = -45$ pC/m, $A_1 = 1.0\times10^{-5}$ J/m^2, $A_2 = 1.0\times10^{-6}$ J/m^2, and $P_{s1}^0 = 7.3$ μC/m^2, $P_{s2}^0 = -2.0$ μC/m^2; (ii) $e_{11}+e_{33} = -45$ pC/m, $A_1 = 4.0\times10^{-5}$ J/m^2, $A_2 = 1.0\times10^{-5}$ J/m^2, and $P_{s1}^0 = 0.73$ μC/m^2, $P_{s2}^0 = 0.29$ μC/m^2; (iii) $e_{11}+e_{33} = 45$ pC/m, $A_1 = 4.0\times10^{-6}$ J/m^2, $A_2 = 3.5\times10^{-6}$ J/m^2, and $P_{s1}^0 = -7.3$ μC/m^2, $P_{s2}^0 = 8.0$ μC/m^2. The results are shown in Figs. 2 and 3.

From these figures, we see that

1) For a small value of U, if the magnitude of surface polarization is suitable, the case both $\omega_1 = 0$, $\omega_2 = 0$ or $\pi/2$ may occur. Then the original HAN cell turns into a planar cell or homeotropic cell effectively, which is similar to the conclusion presented in Ref. [13]. However, if $\omega_1 = 0$, $\omega_2 = \pi/2$ or $\omega_1 = \pi/2$, $\omega_2 = 0$, the cell remains an HAN cell.

2) For a certain value of U (in a certain interval), ω_1 (or ω_2) equals a certain definite value (not including 0 and $\pi/2$), then the effective anchoring of this substrate has a pretilt angle and its maximal value is close to 42° in the cases concerned by these figures above.

3) For a large value of U, if $e_{11}+e_{33} > 0$, we have $\omega_1 = 0$ and $\omega_2 = \pi/2$, then it remains an HAN cell, in which the effective anchoring strengths $A_{1\rm eff}$ and $A_{2\rm eff}$ grow up linearly with

U. However, if $e_{11}+e_{33}<0$, we have $\omega_2=0$ and $\omega_1=\pi/2$. Although the cell remains an HAN cell, it seems that the upper and the lower substrate are placed upside down. The effective anchoring strengths $A_{1\mathrm{eff}}$ and $A_{2\mathrm{eff}}$ also grow up linearly with U.

These results can be directly obtained from Tables 1 and 2 in Section 4. In spite of planar or homeotropic anchoring of a substrate, the effective anchoring may be either planar or homeotropic, or has a pretilt angle especially the magnitude of surface polarization and the value of U are suitable. It means that surface and flexoelectric polarization change the anchoring property of the substrate to produce the effective anchoring energy. Essentially, the influences of surface and flexoelectric polarization on the anchoring property of the substrate in a weak anchoring HAN cell are due to the director deformation of the surface of the substrate. So that, these two polarizations should be considered when investigating the anchoring property of the substrate in detail.

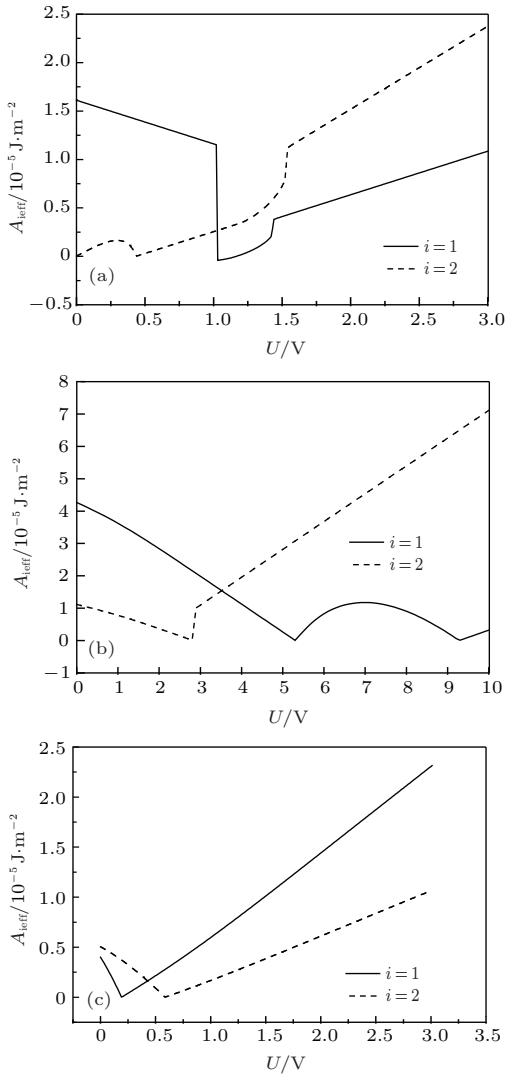


Fig. 2. Variations of the effective anchoring strength with applied voltage. The material parameters of LC are $k_{11}=13.2$ pN, $k_{33}=18.3$ pN, are $\Delta\varepsilon=4.8$. The thickness of NLC cell is $l=10$ μm. Panels (a), (b), and (c) correspond to the three sets of parameters respectively, as given in the text.

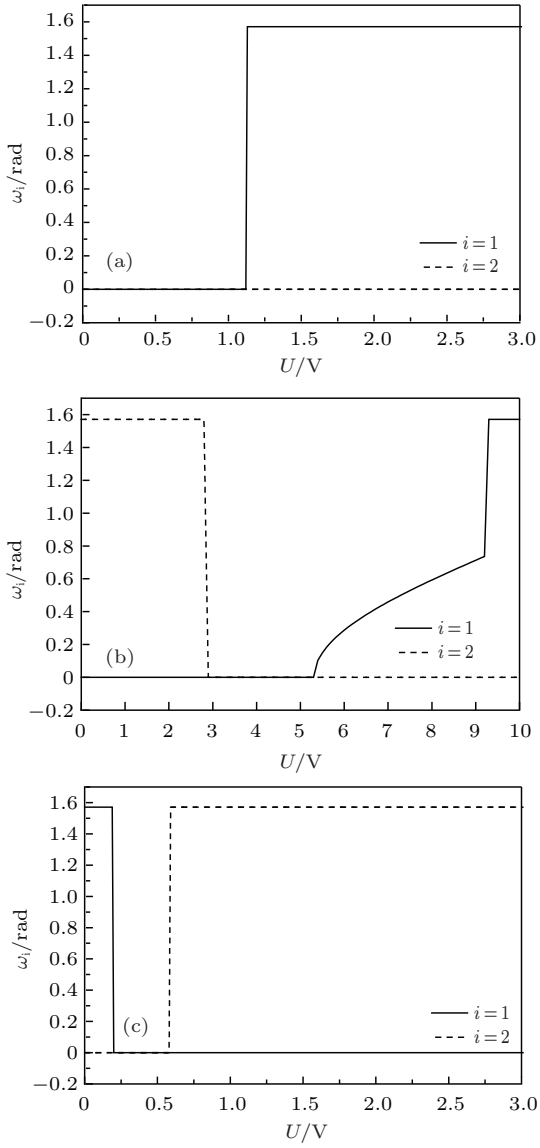


Fig. 3. Variations of tilt angles of the effective anchoring with applied voltage. The material parameters of LC are $k_{11}=13.2$ pN, $k_{33}=18.3$ pN, and $\Delta\varepsilon=4.8$. The thickness of NLC cell is $l=10$ μm. Panels (a), (b), and (c) correspond to the three sets of parameters respectively, as given in the text.

6. Conclusions and discussion

In this paper, we derived the concrete expressions of the effective anchoring energy. Both the effective anchoring strength and the corresponding easy direction are related to the magnitudes of two polarizations as well as the applied voltage. This result is obtained in the case of ignoring the adsorptive ions of the substrate surface. That is to say, the surface polarization may make a contribution to the effective anchoring energy, even in the absence of adsorptive ions, by reason that there is flexoelectric polarization.

In a factual problem, there exist not only surface and flexoelectric polarization but also the adsorptive ions. In this case, the energy term contributed by adsorptive ions as mentioned in Refs. [5], [6], and [8], should be added to the Gibbs free energy. Therefore, our work should be generalized.

Appendix A

Substituting Eq. (6) into Eq. (5), one can obtain

$$\begin{aligned}
&\int_0^l \frac{1}{2}\frac{\partial f_{\rm eff}(\theta)}{\partial\theta}\theta'^2\xi\,{\rm d}z+\int_0^l f_{\rm eff}(\theta)\,\theta'\xi'\,{\rm d}z\\
&-\frac{1}{2}\frac{U_{\rm eff}^2}{\left[\int_0^l \frac{{\rm d}z}{g(\theta)}\right]^2}\int_0^l \frac{\Delta\varepsilon\sin 2\theta}{[g(\theta)]^2}\xi\,{\rm d}z-\frac{U_{\rm eff}}{\int_0^l \frac{{\rm d}z}{g(\theta)}}\left.\frac{\partial U_{\rm eff}}{\partial\alpha}\right|_{\alpha=0}\\
&+\frac{1}{2}\int_0^{\delta_1}\frac{\partial}{\partial\theta}\left[\frac{P_{{\rm s}1z}^2}{g(\theta)}\right]\xi\,{\rm d}z+\frac{1}{2}\int_{l-\delta_2}^{l}\frac{\partial}{\partial\theta}\left[\frac{P_{{\rm s}2z}^2}{g(\theta)}\right]\xi\,{\rm d}z\\
&+\frac{e_{11}+e_{33}}{2}\int_0^{\delta_1}\left\{\frac{\partial}{\partial\theta}\left[\frac{P_{{\rm s}1z}\sin 2\theta}{g(\theta)}\right]\theta'\xi+\frac{P_{{\rm s}1z}\sin 2\theta}{g(\theta)}\xi'\right\}{\rm d}z\\
&+\frac{e_{11}+e_{33}}{2}\int_{l-\delta_2}^{l}\left\{\frac{\partial}{\partial\theta}\left[\frac{P_{{\rm s}2z}\sin 2\theta}{g(\theta)}\right]\theta'\xi+\frac{P_{{\rm s}2z}\sin 2\theta}{g(\theta)}\xi'\right\}{\rm d}z\\
&+\frac{1}{2}A_1\sin 2(\theta_0-\Theta_1)\,\xi_0+\frac{1}{2}A_2\sin 2(\theta_l-\Theta_2)\,\xi_l=0. \qquad ({\rm A1})
\end{aligned}$$

Some terms in Eq. (A1) can be denoted as the following form

$$\left.\frac{\partial U_{\rm eff}}{\partial\eta}\right|_{\eta=0}\approx\frac{e_{11}+e_{33}}{2}\left\{\frac{\sin 2\theta_l}{g(\theta_l)}\xi_l-\frac{\sin 2\theta_0}{g(\theta_0)}\xi_0\right\}, \qquad ({\rm A2})$$

$$\int_0^l f_{\rm eff}(\theta)\,\theta'\xi'\,{\rm d}z=f_{\rm eff}(\theta)\,\theta'\xi\big|_0^l-\int_0^l\frac{\partial}{\partial z}\left[f_{\rm eff}(\theta)\,\theta'\right]\xi\,{\rm d}z, \qquad ({\rm A3})$$

$$\int_0^{\delta_1}\frac{P_{{\rm s}1z}\sin 2\theta}{g(\theta)}\xi'\,{\rm d}z=\frac{P_{{\rm s}1z}\sin 2\theta}{g(\theta)}\xi\Big|_0^{\delta_1}-\int_0^{\delta_1}\frac{\partial}{\partial z}\left[\frac{P_{{\rm s}1z}\sin 2\theta}{g(\theta)}\right]\xi\,{\rm d}z, \qquad ({\rm A4})$$

$$\int_{l-\delta_2}^{l}\frac{P_{{\rm s}2z}\sin 2\theta}{g(\theta)}\xi'\,{\rm d}z=\frac{P_{{\rm s}2z}\sin 2\theta}{g(\theta)}\xi\Big|_{l-\delta_2}^{l}-\int_{l-\delta_2}^{l}\frac{\partial}{\partial z}\left[\frac{P_{{\rm s}2z}\sin 2\theta}{g(\theta)}\right]\xi\,{\rm d}z, \qquad ({\rm A5})$$

$$\int_0^{\delta_1}\frac{\partial}{\partial\theta}\left[\frac{P_{{\rm s}1z}^2}{g(\theta)}\right]\xi\,{\rm d}z\approx\frac{\partial}{\partial\theta}\left[\frac{P_{{\rm s}1z}^2}{g(\theta)}\right]_{\theta=\theta_0}\delta_1\xi_0, \qquad ({\rm A6})$$

$$\int_{l-\delta_2}^{l}\frac{\partial}{\partial\theta}\left[\frac{P_{{\rm s}2z}^2}{g(\theta)}\right]\xi\,{\rm d}z\approx\frac{\partial}{\partial\theta}\left[\frac{P_{{\rm s}2z}^2}{g(\theta)}\right]_{\theta=\theta_l}\delta_2\xi_l. \qquad ({\rm A7})$$

Substituting Eqs. (A2)–(A7) into Eq. (A1), equation (7) and boundary conditions (8) and (9) may be obtained. Here, some terms proportional to δ_1 or δ_2 are ignored because they are very small compared with the other term. The reasons are as follows.

This term containing δ_1 can be written as

$$\begin{aligned}
&\frac{\partial}{\partial\theta}\left[\frac{P_{{\rm s}1z}^2}{g(\theta)}\right]_{\theta=\theta_0}\delta_1\\
&=\left[\frac{2P_{{\rm s}1z}\left(P_{\rm s1}^0 r\sin 2\theta_0\right)}{g(\theta_0)}-\frac{P_{{\rm s}1z}^2\Delta\varepsilon\sin 2\theta_0}{g^2(\theta_0)}\right]\delta_1. \qquad ({\rm A8})
\end{aligned}$$

Comparing it with the term $(e_{11}+e_{33})/2\cdot(P_{{\rm s}1z}\sin 2\theta_0)/g(\theta_0)$, we can obtain

$$\frac{\dfrac{\partial}{\partial\theta}\left[\dfrac{P_{{\rm s}1z}^2}{g(\theta)}\right]_{\theta=\theta_0}\delta_1}{\dfrac{e_{11}+e_{33}}{2}\dfrac{P_{{\rm s}1z}\sin 2\theta_0}{g(\theta_0)}}=\frac{2P_{\rm s1}^0 r-P_{{\rm s}1z}^2\Delta\varepsilon/g(\theta_0)}{\dfrac{e_{11}+e_{33}}{2l}}\frac{\delta_1}{l}, \qquad ({\rm A9})$$

in which the term $(\partial/\partial\theta)\left[P_{{\rm s}1z}^2/g(\theta)\right]_{\theta=\theta_0}\delta_1$ may be neglected with respect to the term $[(e_{11}+e_{33})/2]\cdot[(P_{{\rm s}1z}\sin 2\theta_0)/g(\theta_0)]$, and the term $(\partial/\partial\theta)\left[P_{{\rm s}2z}^2/g(\theta)\right]_{\theta=\theta_l}\delta_2$ may also be neglected compared with the term $[(e_{11}+e_{33})/2]\cdot[(P_{{\rm s}2z}\sin 2\theta_l)/g(\theta_l)]$.

It is very notable that the rigorous expression of $U_{\rm eff}$ is given by

$$\begin{aligned}
U_{\rm eff}=&\,U+\frac{e_1+e_3}{2\Delta\varepsilon}\ln\frac{g(\theta_l)}{g(\theta_0)}+\int_0^{\delta_1}\frac{P_{{\rm s}1z}}{g(\theta)}\,{\rm d}z\\
&+\int_{l-\delta_2}^{l}\frac{P_{{\rm s}2z}}{g(\theta)}\,{\rm d}z. \qquad ({\rm A10})
\end{aligned}$$

However, the latter two terms in Eq. (A10) are neglected when deducing the fundamental equation. If these two terms are considered, the boundary conditions should increase two terms $D_z(\partial/\partial\theta)\left[P_{{\rm s}1z}/g(\theta)\right]_{\theta=\theta_0}\delta_1$ and $D_z(\partial/\partial\theta)\left[P_{{\rm s}2z}/g(\theta)\right]_{\theta=\theta_l}\delta_2$ additionally. Taking the term $D_z(\partial/\partial\theta)\left[P_{{\rm s}1z}/g(\theta)\right]_{\theta=\theta_0}\delta_1$ for example, comparing it with the term $[(e_{11}+e_{33})/2]\cdot D_z\cdot[\sin 2\theta_0/g(\theta_0)]$, we can obtain

$$\frac{D_z\dfrac{\partial}{\partial\theta}\left[\dfrac{P_{{\rm s}1z}}{g(\theta)}\right]_{\theta=\theta_0}\delta_1}{\dfrac{e_{11}+e_{33}}{2}D_z\dfrac{\sin 2\theta_0}{g(\theta_0)}}=\frac{P_{\rm s1}^0 r-P_{{\rm s}1z}\Delta\varepsilon/g(\theta_0)}{\dfrac{e_{11}+e_{33}}{2l}}\frac{\delta_1}{l}. \qquad ({\rm A11})$$

So the term $D_z(\partial/\partial\theta)\left[P_{{\rm s}1z}/g(\theta)\right]_{\theta=\theta_0}\delta_1$ may be neglected. Similarly, the term $D_z(\partial/\partial\theta)\left[P_{{\rm s}2z}/g(\theta)\right]_{\theta=\theta_l}\delta_2$ may also be neglected.

Appendix B

B1. Function D_z of θ_0 and θ_l

According to the constant C for both upper and lower substrates, we have

$$f_{\rm eff}(\theta_0)\,\theta_0'^2-\frac{D_z^2}{g(\theta_0)}=f_{\rm eff}(\theta_l)\,\theta_l'^2-\frac{D_z^2}{g(\theta_l)}. \qquad ({\rm B1})$$

Substituting the boundary conditions Eqs. (8) and (9) into Eq. (B1), we have

$$\begin{aligned}
&\left\{\frac{e\sin 2\theta_0}{g(\theta_0)\sqrt{f_{\rm eff}(\theta_0)}}D_z-\frac{e\sin 2\theta_0}{g(\theta_0)\sqrt{f_{\rm eff}(\theta_0)}}P_{{\rm s}1z}\right.\\
&\left.+\frac{1}{2}\frac{A_1}{\sqrt{f_{\rm eff}(\theta_0)}}\sin 2(\theta_0-\Theta_1)\right\}^2\\
&-\left\{\frac{e\sin 2\theta_l}{g(\theta_l)\sqrt{f_{\rm eff}(\theta_l)}}D_z-\frac{e\sin 2\theta_l}{g(\theta_l)\sqrt{f_{\rm eff}(\theta_l)}}P_{{\rm s}2z}\right.
\end{aligned}$$

$$-\frac{1}{2}\frac{A_2}{\sqrt{f_{\rm eff}(\theta_l)}}\sin 2(\theta_l-\Theta_2)\Bigg\}^2 - \frac{g(\theta_l)-g(\theta_0)}{g(\theta_0)g(\theta_l)}D_z^2=0, \tag{B2}$$

where $e=(e_{11}+e_{33})/2$. Introducing the following quantities: $\lambda_1 = e\sin 2\theta_0/(g(\theta_0)\sqrt{f_{\rm eff}(\theta_0)})$, $\lambda_2 = e\sin 2\theta_l/(g(\theta_l)\sqrt{f_{\rm eff}(\theta_l)})$,

$$\sigma=\frac{g(\theta_l)-g(\theta_0)}{g(\theta_0)g(\theta_l)},$$

$$\tau_1=-\frac{e\sin 2\theta_0}{g(\theta_0)\sqrt{f_{\rm eff}(\theta_0)}}P_{\rm s1z}+\frac{1}{2}\frac{A_1}{\sqrt{f_{\rm eff}(\theta_0)}}\sin 2(\theta_0-\Theta_1),$$

and

$$\tau_2=-\frac{e\sin 2\theta_l}{g(\theta_l)\sqrt{f_{\rm eff}(\theta_l)}}P_{\rm s2z}+\frac{1}{2}\frac{A_2}{\sqrt{f_{\rm eff}(\theta_l)}}\sin 2(\theta_l-\Theta_2),$$

equation (B2) can be simplified into the following form:

$$\left(\lambda_1^2-\lambda_2^2-\sigma\right)D_z^2+2(\lambda_1\tau_1-\lambda_2\tau_2)D_z+\left(\tau_1^2-\tau_2^2\right)=0. \tag{B3}$$

From Eq. (B3) the expression of D_z is obtained as

$$D_z=\frac{-(\lambda_1\tau_1-\lambda_2\tau_2)\pm\sqrt{(\lambda_1\tau_2-\lambda_2\tau_1)^2+\sigma\left(\tau_1^2-\tau_2^2\right)}}{\lambda_1^2-\lambda_2^2-\sigma}. \tag{B4}$$

B2. Expression of $A_{1\rm eff}$ for $\omega_1=\sin^{-1}R_1$

For $\Theta_1=0$, equation (27) can be simplified into

$$A_1+\frac{2e}{g(\omega_1)}\left(D_z-P_{\rm s1}^0+P_{\rm s1}^0 r\sin^2\theta_0\right)=0, \tag{B5}$$

and equation (B2) can be simplified into

$$\frac{\sin^2 2\theta_0}{f_{\rm eff}(\theta_0)}\left\{\frac{e}{g(\theta_0)}\left(D_z-P_{\rm s1}^0-P_{\rm s1}^0 r\sin^2\theta_0\right)+\frac{1}{2}A_1\right\}^2 - \frac{\sin^2 2\theta_l}{f_{\rm eff}(\theta_l)}\left\{\frac{e}{g(\theta_l)}\left(D_z-P_{\rm s2}^0-P_{\rm s2}^0 r\sin^2\theta_l\right)-\frac{1}{2}A_2\right\}^2 - \frac{g(\theta_l)-g(\theta_0)}{g(\theta_0)g(\theta_l)}D_z^2=0. \tag{B6}$$

From Eqs. (24) and (28), we need to know the expression of $\left.\frac{\partial D_z}{\partial\theta_0}\right|_{\theta_0=\omega_1}$ to obtain the expression of $A_{1\rm eff}$ for $\omega_1=\sin^{-1}R_1$. So, we deduce the expression of $\left.\frac{\partial D_z}{\partial\theta_0}\right|_{\theta_0=\omega_1}$ first by using Eq. (B6),

$$\left.\frac{\partial D_z}{\partial\theta_0}\right|_{\theta_0=\omega_1}=-\frac{D_z\Delta\varepsilon\sin\omega_1}{2\left\{\left(\frac{1}{g(\theta_l)}-\frac{1}{g(\omega_1)}\right)\pm\frac{\sin 2\theta_l}{\sqrt{f_{\rm eff}(\theta_l)}}\sqrt{\frac{1}{g(\theta_l)}-\frac{1}{g(\omega_1)}}\right\}g^2(\omega_1)}. \tag{B7}$$

Equation (B7) contains θ_l, which can be determined by the following equation obtained by using Eqs. (B5) and (B6) for $\theta_0=\omega_1$:

$$\frac{\sin^2 2\theta_l}{f_{\rm eff}(\theta_l)}\left\{\frac{e}{g(\theta_l)}\left(D_z-P_{\rm s2}^0-P_{\rm s2}^0 r\sin^2\theta_l\right)-\frac{1}{2}A_2\right\}^2-\frac{g(\theta_l)-g(\omega_1)}{g(\omega_1)g(\theta_l)}D_z^2=0. \tag{B8}$$

Substituting Eq. (B7) into Eq. (28), the expression of $A_{1\rm eff}$ for $\omega_1=\sin^{-1}R_1$ can be obtained as

$$A_{1\rm eff}=\frac{\left[A_1-\frac{e_1+e_3}{\varepsilon_\perp}\left(P_{\rm s1}^0-D_z\right)\right]\left[A_1-\frac{e_1+e_3}{\varepsilon_\parallel}\left[P_{\rm s1}^0(1+r)-D_z\right]\right]}{\frac{e_1+e_3}{2}\left(\frac{1}{\varepsilon_\perp}-\frac{1}{\varepsilon_\parallel}\right)\left[D_z-P_{\rm s1}^0+\frac{\varepsilon_\perp}{\Delta\varepsilon}P_{\rm s1}^0 r\right]^2}\left(D_z-P_{\rm s1}^0+\frac{\varepsilon_\perp}{\Delta\varepsilon}P_{\rm s1}^0 r+\Delta_1\right), \tag{B9}$$

where

$$\Delta_1=\frac{D_z}{2\left[\left(\frac{g(\omega_1)}{g(\theta_l)}-1\right)\pm\frac{e\sin 2\theta_l}{g(\theta_l)}\sqrt{\frac{g(\omega_1)}{f_{\rm eff}(\theta_l)}}\left(\frac{g(\omega_1)}{g(\theta_l)}-1\right)^{1/2}\right]}. \tag{B10}$$

The selection of the sign of "±" should make $A_{1\rm eff}$ minimum and $A_{1\rm eff}\geq 0$.

B3. Expression of $A_{2\rm eff}$ for $\omega_2=\sin^{-1}R_2$

Adopting the same method to solve the expression of $A_{1\rm eff}$ for $\omega_1=\sin^{-1}R_1$, the expression of $A_{2\rm eff}$ for $\omega_2=\sin^{-1}R_2$ can be obtained as

$$A_{2\rm eff}=\frac{\left[-A_2+\frac{e_{11}+e_{33}}{\varepsilon_\perp}\left(D_z-P_{\rm s2}^0\right)\right]\left[A_2-\frac{e_{11}+e_{33}}{\varepsilon_\parallel}\left[D_z-P_{\rm s2}^0(1+r)\right]\right]}{\frac{e_{11}+e_{33}}{2}\left(\frac{1}{\varepsilon_\perp}-\frac{1}{\varepsilon_\parallel}\right)\left[D_z-P_{\rm s2}^0+\frac{\varepsilon_\perp}{\Delta\varepsilon}P_{\rm s2}^0 r\right]^2}\left(D_z-P_{\rm s2}^0+\frac{\varepsilon_\perp}{\Delta\varepsilon}P_{\rm s2}^0 r+\Delta_2\right), \tag{B11}$$

where

$$\Delta_2 = \frac{D_z}{2\left[\left(\frac{g(\omega_2)}{g(\theta_0)} - 1\right) \pm \frac{e\sin 2\theta_0}{g(\theta_0)}\sqrt{\frac{g(\omega_2)}{f_{\text{eff}}(\theta_0)}}\left(\frac{g(\omega_2)}{g(\theta_0)} - 1\right)^{1/2}\right]}. \tag{B12}$$

The selection of the sign of "±" should make $A_{2\text{eff}}$ minimum and $A_{2\text{eff}} \geq 0$.

Note that Δ_1 or Δ_2 may be seen as a modification of $A_{1\text{eff}}$ or $A_{2\text{eff}}$ due to $\frac{\partial D_z}{\partial \theta_0}\Big|_{\theta_0=\omega_1} \neq 0$ or $\frac{\partial D_z}{\partial \theta_l}\Big|_{\theta_l=\omega_2} \neq 0$. However, we find that this modification is so small (the value is only on the order of 10^{-3}) that it can be neglected.

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