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Flexoelectric-Induced Voltage Shift in Hybrid Aligned Nematic Liquid Crystal Cell*

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Abstract *Flexoelectric-induced voltage shift in a weak anchoring hybrid aligned nematic liquid crystal cell is investigated theoretically. Based on the elastic theory of liquid crystal and the variation method, the equations for the bulk and the boundary of the cell are derived. By computer simulation, the dependence of the shift voltage on the sum of the flexoelectric coefficients and the anchoring energy strength is obtained. As a result, a novel method to determine the sum of the flexoelectric coefficients by measuring the shift voltage is put forward.*

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Key words: flexoelectric, voltage shift, hybrid aligned nematic, shift voltage, variation method

Liquid crystal display (LCD) technology has always been a major concern in flat panel display (FPD) industry since the twisted nematic liquid crystal display (TN-LCD) mode[1] was brought forward and this technology is increasingly developed and improved better and better. The principal part of an LCD device is LCD cell which consists of LC layer contained between two pre-treated substrates.[2] LCD is passive display, and it depends on LC layer to modulate the incident linear polarized light when an external voltage is applied. The orientational deformation of LC (including the splay, twist and bend deformation) leads to the variation of transmittance. For the pear-shaped or the banana-shaped LC molecules with permanent dipoles, the flexoelectric effect[3] is induced for the splay or the bend deformation, which can realize the switching from the "defect state" to the "defect-free state" in zenithal bistable device (ZBD)[4] and induce a kind of two-dimensional electroconvection at ultralow electric frenquency.[5] In this case the actual voltage exerted to the LC layer will change due to the flexoelectric effect when an external voltage is applied. In other words, a flexoelectric-induced shift voltage will generate in this case.

In 1998, Takahashi *et al.*[6] found that electro-optical characteristics of hybrid aligned nematic (HAN) cell have a deviation under considering the flexoelectric effect relative to the case with ignoring it which was found in Ref. [7] with the charged impurities in LC material. The corresponding voltage of deviation is called as the shift voltage. By fitting experimental electro-optical characteristics of hybrid aligned nematic (HAN) cells with numerical simulations, they still gave the values of the flexoelectric coefficients. Kirkman *et al.*[8] proposed a continuum modeling of HAN cell to study the optical response and the flexoelectric-induced voltage shift. They mainly adopted the method of numerical simulation and compared their results with the experimental data in Ref. [6]. This implies that the flexoelectric coefficients can be obtained by measuring the shift voltage.

Since the flexoelectric effect was proposed, to determine the influence of flecoelectric effect, many researchers adopted different methods to measure the flexoelectric coefficients.[6,9−13] However, for the same LC material, they gave different results. Therefore, the precise measurement of the flexoelectric coefficients is very important to display characteristics of LCD, especially the ZBD. In this paper, we bring forward the design of determining the sume of flexoelectric coefficients based on the theoretical analysis of the shift voltage induced flexoelectric effect.

Our selected weak anchoring HAN cell structure and the Cartesian coordinate system are shown in Fig. 1. A nematic liquid crystal (NLC) is filled in the cell, in which the LC molecules at the lower substrate and the upper substrate orient along the x direction and the z direction, respectively. LC molecules gradually orient along the z direction from the lower substrate to the upper substrate without an applied voltage. The original point of Cartesian coordinate system is laid in the plane of the lower substrate. The anchoring energy strengths corresponding to the lower and upper substrate are A_0 and A_l, respectively. An external voltage is applied to the cell perpen-

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dicular to these two substrates, and the electric potential at the lower substrate is zero.

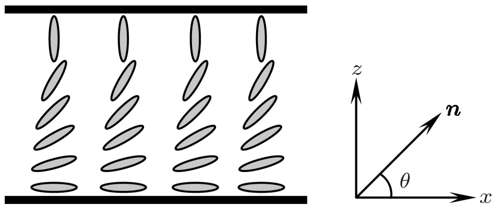

Fig. 1 Structure of HAN cell and the Cartesian coordinate system.

The HAN cell can be seen a sealed system. If there are no ionic impurities in LC, there is no free charge in the system. Maxwell's equations then reduce to $\boldsymbol{\nabla}\times\boldsymbol{D}=0$ and $\boldsymbol{\nabla}\cdot\boldsymbol{D}=0$.[14] Because the electric field is along the z direction, the director deformation (including the splay and bend deformation) in the HAN cell is only in the xoz plane and the tilt angle between the director $\boldsymbol{n}$ and the x axis is θ which is only dependent on the coordinate z. The z component of electric displacement vector is a constant within the whole cell. Considering the polarization due to the flexoelectric effect, the z component of electric displacement vector can be written as

$$\boldsymbol{D}_z = g\,(\theta)\,E_z + P_{fz}, \tag{1}$$

where E_z and P_{fz} are the components of $\boldsymbol{E}$ and $\boldsymbol{P}_f$, $g(\theta)=\varepsilon_0(\varepsilon_\perp+\Delta\varepsilon\sin^2\theta)$, ε_0 is the permittivity of vacuum, $\varepsilon_\perp$ is the permittivity across the axis of LC, $\Delta\varepsilon$ is the anisotropy of the permittivity, and

$$\boldsymbol{P}_f = e_{11}\boldsymbol{n}(\nabla\cdot\boldsymbol{n}) + e_{33}(\nabla\times\boldsymbol{n})\times\boldsymbol{n}, \tag{2}$$

where e_{11} and e_{33} are the splay and bend flexoelectric coefficients.[3] The electric field is therefore

$$E_z = \frac{D_z - P_{fz}}{g(\theta)}. \tag{3}$$

Integrating the electric field to find the electric potential (the voltage value applied to the cell)

$$-V = \int_0^l E_z\,\mathrm{d}z = D_z\int_0^l \frac{\mathrm{d}z}{g(\theta)} - \int_0^l \frac{P_{fz}}{g(\theta)}\mathrm{d}z. \tag{4}$$

The electric potential now consists of two terms, the first being due to dielectric effect and the second due to the flexoelectric effect. The actual voltage exerted to the LC layer to control the LC molecules deformation is the first term. The second term plays a role in the voltage shift. The analytic expression of the shift voltage induced by the flexoelectric effect can be simplified as[14]

$$V_{\text{shift}} = \int_0^l \frac{P_{fz}}{g(\theta)}\mathrm{d}z = \frac{e_{11}+e_{33}}{2\varepsilon_0\Delta\varepsilon}\ln\frac{g(\theta_l)}{g(\theta_0)}, \tag{5}$$

where θ_0 and θ_l are the tilt angles for the lower and the upper substrate, respectively.

From (5), one can see that the shift voltage is dependent on both the tilt angles on the surface of two substrates and the flexoelectric coefficients of LC material. For the special case, strong anchoring HAN cell, the variation of the shift voltage with the sum of the flexoelectric coefficients is linear. For weak anchoring HAN cell, however, the variation of the shift voltage with the sum of the flexoelectric coefficients can be obtained based on the determinate tilt angles. As a result, solving the tilt angles is the key point. Therefore, the equilibrium equations for the weak anchoring HAN cell must be given firstly.

The total free energy density of this system consists of the elastic, dielectric, flexoelectric and surface contributions:

$$f = f_{\text{elas}} + f_{\text{diel}} + f_{\text{flexo}} + f_{s0} + f_{sl}, \tag{6}$$

where

$$f_{\text{elas}} = \frac{1}{2}f(\theta)\Big(\frac{\mathrm{d}\theta}{\mathrm{d}z}\Big)^2, \tag{7}$$

$$f_{\text{diel}} = -\frac{1}{2}g(\theta)\Big(\frac{\mathrm{d}\varphi}{\mathrm{d}z}\Big)^2, \tag{8}$$

$$f_{\text{flexo}} = \frac{1}{2}(e_{11}+e_{33})\sin(2\theta)\frac{\mathrm{d}\theta}{\mathrm{d}z}\frac{\mathrm{d}\varphi}{\mathrm{d}z}, \tag{9}$$

$$f_{s0} = \frac{1}{2}A_0\sin^2(\theta_0-\Theta_0), \tag{10}$$

$$f_{sl} = \frac{1}{2}A_l\sin^2(\theta_l-\Theta_l), \tag{11}$$

where $f(\theta) = k_{11}\cos^2\theta + k_{33}\sin^2\theta$, k_{11} and k_{33} are the splay and bend elastic constant, Θ_0 and Θ_l are the pretilt angles of the lower and upper substrate, φ is the electric potential of LC layer. Substituting (6) into the Euler–Lagrange equations[15] or adopting the variational method,[16–17] one can easily obtain the bulk equilibrium equations of the tilt angle and the electric potential as shown in the following

$$f'(\theta)\Big(\frac{\mathrm{d}\theta}{\mathrm{d}z}\Big)^2 + 2f(\theta)\frac{\mathrm{d}^2\theta}{\mathrm{d}z^2} + g'(\theta)\Big(\frac{\mathrm{d}\varphi}{\mathrm{d}z}\Big)^2 + (e_{11}+e_{33})\sin(2\theta)\frac{\mathrm{d}^2\varphi}{\mathrm{d}z^2} = 0, \tag{12}$$

$$g'(\theta)\Big(\frac{\mathrm{d}\theta}{\mathrm{d}z}\Big)\Big(\frac{\mathrm{d}\varphi}{\mathrm{d}z}\Big) + g(\theta)\Big(\frac{\mathrm{d}^2\varphi}{\mathrm{d}z^2}\Big) - (e_{11}+e_{33})\cos(2\theta)\Big(\frac{\mathrm{d}\theta}{\mathrm{d}z}\Big)^2 - \frac{1}{2}(e_{11}+e_{33})\sin(2\theta)\Big(\frac{\mathrm{d}^2\theta}{\mathrm{d}z^2}\Big) = 0, \tag{13}$$

and the boundary conditions for the lower and upper substrate

$$f(\theta_0)\frac{\mathrm{d}\theta}{\mathrm{d}z}\Big|_{z=0} + \frac{1}{2}(e_{11}+e_{33})\sin(2\theta_0)\frac{\mathrm{d}\varphi}{\mathrm{d}z}\Big|_{z=0} - \frac{1}{2}A_0\sin[2(\theta_0-\Theta_0)] = 0, \tag{14}$$

$$f(\theta_l)\frac{\mathrm{d}\theta}{\mathrm{d}z}\Big|_{z=l} + \frac{1}{2}(e_{11}+e_{33})\sin(2\theta_l)\frac{\mathrm{d}\varphi}{\mathrm{d}z}\Big|_{z=l} + \frac{1}{2}A_l\sin[2(\theta_l-\Theta_l)] = 0. \tag{15}$$

Equations (12), (13), (14), and (15) are the fundamental equations to determine the tilt angles θ_0 and θ_l. These four equations are all differential equations, then obtaining the analytic solution of θ_0 and θ_l is very difficult. So, we use the numerical simulation to determine θ_0 and θ_l.

Our adopted calculation method is the finite-difference iterative method used in Refs. [18]–[19]. Dividing the whole LC layer into N ($N = 100$) sub-layers, the upper substrate and the lower substrate correspond to the N-th sub-layer and the 1st sub-layer. The forms of the finite-difference for the tilt angle θ and the electric potential φ are

$$\theta_i' = \frac{-3\theta_i + 4\theta_{i+1} - \theta_{i+2}}{2h}, \quad \varphi_i' = \frac{-3\varphi_i + 4\varphi_{i+1} - \varphi_{i+2}}{2h}, \quad (i = 1), \tag{16}$$

$$\theta_i' = \frac{\theta_{i-2} - 4\theta_{i-1} + 3\theta_i}{2h}, \quad \varphi_i' = \frac{\varphi_{i-2} - 4\varphi_{i-1} + 3\varphi_i}{2h}, \quad (i = N), \tag{17}$$

$$\theta_i' = \frac{\theta_{i+1} - \theta_{i-1}}{2h}, \quad \theta_i'' = \frac{\theta_{i-1} - 2\theta_i + \theta_{i+1}}{h^2}, \quad (1 < i < N), \tag{18}$$

$$\varphi_i' = \frac{\varphi_{i+1} - \varphi_{i-1}}{2h}, \quad \varphi_i'' = \frac{\varphi_{i-1} - 2\varphi_i + \varphi_{i+1}}{h^2}, \quad (1 < i < N), \tag{19}$$

where $h = l/N$ is the distance of an LC sub-layer.

Substituting the forms of the finite-difference into the equations and the boundary conditions, one can obtain the iterative equations of the tilt angle θ and the electric potential ϕ. Through programming calculation, the director profile in the whole LC layer can be confirmed and θ_0 and θ_l are certainly contained in it.

Distributions of director in HAN cell for different sum of flexoelectric coefficients e_{11} and e_{33} under an external voltage 5 V at three anchoring energy strengths (a) $A_0 = A_l$=1.0×10^{-6} J/m^2, (b) $A_0 = A_l$=1.0×10^{-5} J/m^2, (c) $A_0 = A_l$=1.0×10^{-4} J/m^2 are shown in Fig. 2. The variations of shift voltage induced flexoelectric effect with the sum of the flexoelectric coefficients e_{11} and e_{33} under an external voltage 5 V for different anchoring energy strengths are shown in Fig. 3. The material parameters of LC are: k_{11}=6.2×10^{-12} N, k_{33}=8.3×10^{-12} N, $\Delta\varepsilon = 5.2$, $\varepsilon_\perp = 5.3$. Thickness of HAN cell is l=1.0×10^{-5} m. Anchoring energy strengths of the lower and upper substrate are assumed to be uniform and take different values $A_0 = A_l$=1.0×10^{-4} J/m^2, 1.0×10^{-5} J/m^2, 1.0×10^{-6} J/m^2.

From Fig. 3, the shift voltage is clearly dependent on both the sum of the flexoelectric coefficients and the anchoring energy strengths. For the case of strong anchoring, i.e. $A_0 = A_l$=1.0×10^{-4} J/m^2, the variation between the shift voltage and the sum of the flexoelectric coefficients is linear from a negative value to a positive value with the increase of the sum of the flexoelectric coefficients. For the case of weak anchoring, however, the shift voltage increases first and then decreases with the increase of the sum of the flexoelectric coefficients, and under a certain range of the sum of the flexoelectric coefficients the shift voltage equals to zero,

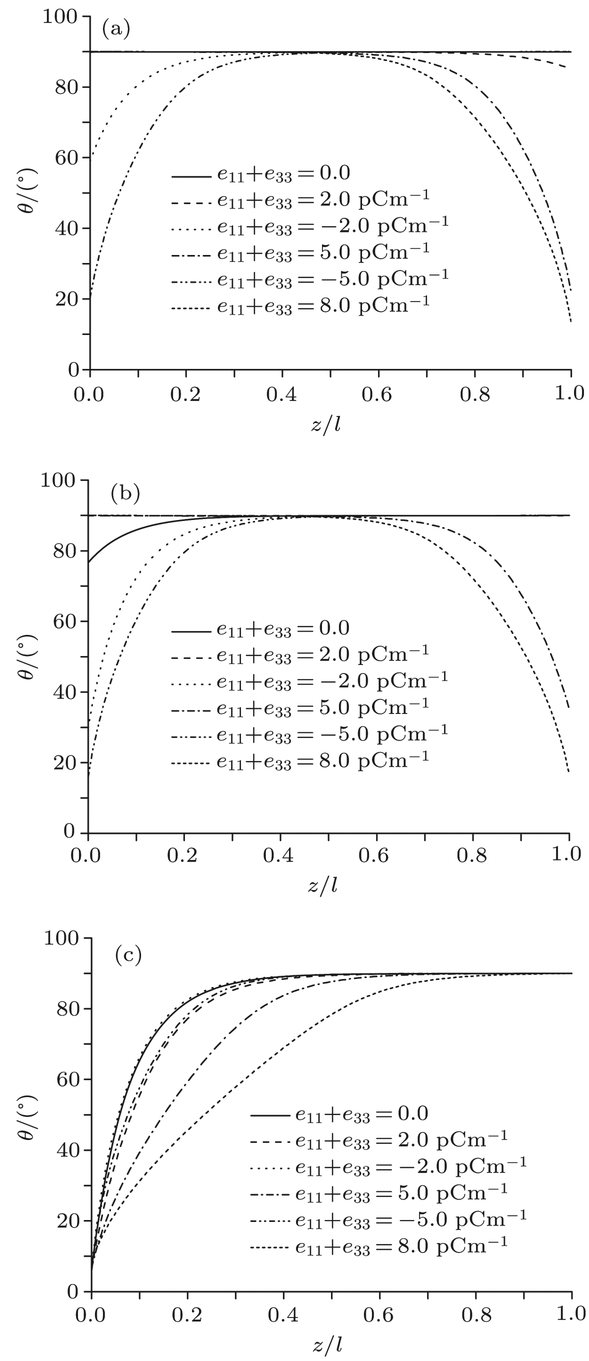

Fig. 2 Distribution of director in HAN cell for different sum of flexoelectric coefficients e_{11} and e_{33} at three anchoring energy strengths (a) $A_0 = A_l$=1.0×10^{-6} J/m^2, (b) $A_0 = A_l$=1.0×10^{-5} J/m^2, (c) $A_0 = A_l$=1.0×10^{-4} J/m^2.

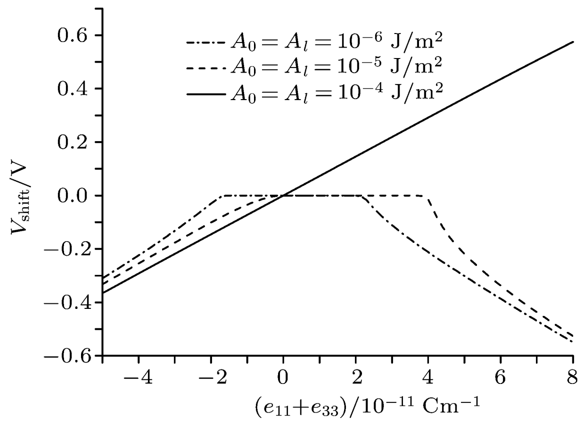

Fig. 3 Dependence of $V_{\rm shift}$ on $(e_{11}+e_{33})$ with different anchoring energy strengths.

wihch means that the actual electric potential applied to the LC layer is just the voltage exerted to HAN cell. The inherent mechanism of flexoelectric-induced voltage shift is distribution of director. From Fig. 2, one can see that distributions of director exists remarkable difference for different anchoring energy strengths and sum of flexoelectric coefficients, which results in the different variations of shift voltage with the sum of the flexoelectric coefficients. As a result, the sum of the flexoelectric coefficients can be determined by comparing the shift voltage obtained from the experiment and the theory.

According to the configurations on the LC material and the HAN cell, we can calculate the transmittance under an external voltage 5 V without considering the flexoelectric effect by the method used in Ref. [7]. During experiment, we need apply a voltage to make the transmittance to attain the above theoretical value. The difference between the applied voltage value and 5 V is the shift voltage.

In this paper, we analyzed theoretically the flexoelectric-induced voltage shift in a weak anchoring HAN cell. By numerical simulation, the dependence of the shift voltage on the sum of the flexoelectric coefficients and the anchoring energy strength was obtained. A novel method to determine the sum of the flexoelectric coefficients through measuring the shift voltage was put forward and it would have a hope to be applied in the future research.

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