Determining the sum of flexoelectric coefficients in nematic liquid crystals by the capacitance method*

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A detailed theoretical analysis of determining the sum of flexoelectric coefficients in nematic liquid crystals using the capacitance method is given. In the strong anchoring parallel aligned nematic (PAN) and hybrid aligned nematic (HAN) cells, the dependences of the capacitance on the sum of flexoelectric coefficients and the applied voltage are obtained by numerical simulations, and the distributions of the director and the electric potential for different applied voltages and flexoelectric coefficients are also given. Based on this theoretical analysis, we propose an experimental design for measuring the capacitance of a liquid crystal cell using the improved precision LCR meter E4980A (Agilent). Through comparing the experimental data with the simulated results, the sum of flexoeletric coefficients can be determined.

Keywords: flexoelectricity, capacitance, parallel aligned nematic and hybrid aligned nematic liquid crystals

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1. Introduction

Flexoelectricity in nematic liquid crystals (NLCs) is a very important material property for the polar pear- or banana-shaped molecules with permanent dipole moment and for non-polar molecules with quadrupole moment.[1] For the polar pear- or banana-shaped molecules, flexoelectric polarization $\boldsymbol{P}$ can arise when the average molecular orientation or director $\boldsymbol{n}$ is subjected to splay or bend deformation, expressed as[2]

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

where e_{11} and e_{33} are the splay and the bend flexoelectric coefficients, respectively. The distortion-induced polarization is called the direct flexoelectric effect, which can affect the energy of the system and result in stable blue phase in chiral liquid crystals[3] and which can form an electro-mechanical transducer to realize the conversion between mechanical and electrical energies.[4] In addition, the converse flexoelectric effect will appear when an external electric field is applied to the liquid crystal layer. There is a coupling between the polarization and the applied electric field, which can induce the deformation of the director to result in the variation of the optical transmissivity. This effect has been exploited in electro-optical devices,[5–7] especially in the zenithal bistable device (ZBD).[5] All of these applications of the flexoelectric effect mentioned above are closely related to the flexoelectric coefficients in the theoretical analysis and, therefore, the specific flexoelectric coefficients are required, which promotes researchers to accurately measure them.

Since Meyer gave the expression of the flexoelectric polarization in 1969, many methods[8–25] to determine the flexoelectric coefficients have been proposed by different research groups. These methods can be divided into two categories: direct and indirect methods, which make use of the direct and the converse flexoeletric effects, respectively. The direct method is based on the measurement of the flexoelectric polarization induced by the deformation of the liquid crystal through a pressure pulse or a heat pulse.[8] The indirect method is based on the interaction between the flexoelectric polarization and the electric field, which affects the optical phase difference,[10,13] the guided mode structure,[14] etc. when a deformation is generated in the liquid crystal layer. For a parallel orientated liquid crystal layer, the effect of flexoelectricity in the Fréedericksz transition can go back at least as far as Deuling.[10], who suggested measuring the optical phase difference to determine the flexoelectric coefficients in a magnetic field rather than in an electric field. However, the magnetic field is inconvenient to be applied to the liquid crystal layer relative to the electric field, and the electric field can be easily controlled by the driven signals. At the same time, Brown and Mottram[11] investigated in detail the effect of flexoelectricity in the Fréedericksz transition, where they considered the dynamic response process. In fact, the response of a liquid crystal display is very fast, at the scale of millisecond, and the liquid crystal system can reach the equilibrium state in short time and some effect can remain. Therefore, it is necessary to consider the changes at the equilibrium state for a

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certain voltage applied to the liquid crystal cell. In addition to these influences of the flexoelectric effect, the capacitance of the liquid crystal cell can also be changed by the flexoelectric effect, which is the motivation of this paper.

With the help of the electric current produced by periodic mechanical flexing of the bent-core NLC bounding surfaces, a direct method was presented by Harden *et al.*[15] They drew a conclusion that the flexoelectric coefficients in bent-core NLCs are three orders of magnitude larger than those in the conventional calamitic (rod-shaped) nematics. To demonstrate the feasibility of the method, a standard calamitic nematic liquid crystal, 4-cyano-4'-npentyl-biphenyl (5CB), was measured to obtain the same magnitude as that in the previous reports. Using the indirect method of polarization-induced flexing to measure the flexoelectric coefficients of the bent-core NLCs, they reached a coincident conclusion with that of the direct method.[16]

However, that result was questioned by other groups. Firstly, Kumar *et al.* adopted the indirect method proposed by Helfrich[26] to measure the flexoelectric coefficients of two bent-core NLCs, which are of the usual order of magnitude as that in calamitic.[21] Secondly, Castles *et al.* proved that the flexoelectric coefficients in NLCs have a clear fundamental limit to the conventional order of magnitude from the conservation of energy considerations.[27,28] They obtained the difference of flexoelectric coefficients of 5CB for the conventional order of magnitude[25] using the indirect method of measuring the chiral flexoeletro-optical property to the uniform lying helix (ULH) structure proposed by Patel *et al.*[29] The indirect method based on the flexoelectro-optical property in NLCs or chiral NLCs exhibit some degree of uncertainty (for example, the anchoring strength of the substrate, the interaction between the NLC molecules and the chiral additive, the measurement accuracy of the instrument, and so on), which leads to the measurement discrepancy of the flexoelectric coefficients, even for the same material. To eliminate this influence, we suggest that the strong anchoring parallel aligned nematic (PAN) or hybrid aligned nematic (HAN) cell filled in the pure insulating NLCs can be used to measure its capacitance. Although we do not present a concrete measurement in this paper, the experimental design of the measurement is listed in detail and the influences of the flexoelectric effect on the capacitances of the PAN and the HAN cells are also analyzed in detail theoretically. If the measurement can be done and comparing the experimental results with the theoretical analysis, then the sum of the flexoelectric coefficients can be determined.

The arrangement of this paper is as follows. Firstly, in Section 2 the analytical expressions of the capacitances in the PAN and the HAN cells are deduced on the basis of the continuum theory. Secondly, in Section 3 we calculate the capacitance for each cell at a fixed applied voltage or a fixed flexoelectric coefficient when the flexoelectric coefficient or the applied voltage takes different values, we also calculate the distributions of the director and the electric potential. Thirdly, in Section 4 an experimental design for measuring the capacitance of the liquid crystal cell using an improved precision LCR meter E4980A (Agilent) is proposed. Finally, a significant discussion and conclusion are given in Section 5.

2. Principle

A liquid crystal (LC) cell may be seen as a capacitor from its configuration. However, unlike other fixed capacitors, the capacitance of the LC cell is tunable with different applied voltages. The main cause that induces the capacitance change of the LC cell is that the deformation of the director leads to the variation of the effective dielectric constant in the whole LC layer. The flexoelectric effect can influence the director, and it is natural to influence the capacitance of the LC cell. Therefore, if one wants to understand this influence, a theoretical analysis and numerical simulation must be given. In this section, we analyze two kinds of LC cells, PAN and HAN cells, and obtain the expressions for the capacitances of these two cells. We will discuss the numerical simulation in the following section.

2.1. PAN cell

Consider NLCs confined between two pretreated identical substrates located at $z = 0$ and $z = l$, respectively, where the z axis is normal to the plane of the substrate. The NLCs near the two substrate surfaces are anchored strongly on the planes. The director $\boldsymbol{n}$ of the LC can be described by the tilt angle θ between the preferred orientation of the NLC molecules and the plane, and the tilt angle is only dependent on the coordinate z.

If there are no ionic impurities in the NLCs, then there is no free charge in the system. Maxwell's equations then reduce to $\nabla \times \boldsymbol{D} = 0$ and $\nabla \cdot \boldsymbol{D} = 0$. Considering the polarization due to the flexoelectric effect, we can write the z component of the electric displacement vector as

$$D_z = g(\theta) E_z + P_z, \tag{2}$$

where E_z and P_z are the components of $\boldsymbol{E}$ and $\boldsymbol{P}$, $g(\theta) = \varepsilon_0 \left(\varepsilon_\perp + \Delta\varepsilon \sin^2 \theta\right)$ is the effective permittivity,[30] ε_0 is the permittivity of vacuum, $\varepsilon_\perp$ is the permittivity across the axis of the LC, $\Delta\varepsilon = \varepsilon_\parallel - \varepsilon_\perp$ is the anisotropy of the permittivity, and $\varepsilon_\parallel$ is the permittivity along the axis of the LC. From Eq. (2), the expression of external applied voltage U can be written as

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

and the distribution of electric potential φ in the liquid crystal layer is given by

$$\frac{\mathrm{d}\varphi}{\mathrm{d}z} = \frac{P_z}{g(\theta)} - \frac{(A - U)}{g(\theta) \int_0^l 1/g(\theta) \mathrm{d}z}, \tag{4}$$

where

$$A = \frac{e_{11}+e_{33}}{2\varepsilon_0\Delta\varepsilon}\ln\frac{g(\theta_l)}{g(\theta_0)}$$

is the electric potential induced by the flexoelectric effect,[31–33] with θ_0 and θ_l being the tilt angles of the lower and the upper substrates, respectively.

Without the external applied voltage, the original equilibrium state can be achieved by the interaction among the LC molecules. The original equilibrium state is broken when an external voltage U perpendicular to these two substrates, with zero electric potential at the lower substrate, is applied to the cell. A new equilibrium state appears because of the action among the dielectric energy, the elastic energy, and the flexoelectric-induced energy. In this case, the free energy per unit area substrate is given by

$$F = \int_0^l (f_{\text{elas}} + f_{\text{diel}} + f_{\text{flex}})\,\mathrm{d}z, \tag{5}$$

where f_{elas}, f_{diel}, and f_{flex} are the elastic, the dielectric, and the flexoeletric free energy densities, respectively. The total free energy density can be written as

$$\begin{aligned} f &= f_{\text{elas}} + f_{\text{diel}} + f_{\text{flex}} \\ &= \frac{1}{2}f(\theta)\left(\frac{\mathrm{d}\theta}{\mathrm{d}z}\right)^2 - \frac{1}{2}g(\theta)\left(\frac{\mathrm{d}\varphi}{\mathrm{d}z}\right)^2 \\ &\quad - \frac{e_{11}+e_{33}}{2}\sin(2\theta)\left(\frac{\mathrm{d}\theta}{\mathrm{d}z}\right)\left(\frac{\mathrm{d}\varphi}{\mathrm{d}z}\right), \end{aligned} \tag{6}$$

where $f(\theta) = k_{11}\cos^2\theta + k_{33}\sin^2\theta$.

By substituting Eq. (6) into the Euler equation,[34] we can easily obtain two coupled differential equations at the equilibrium state for the tilt angle and the potential

$$\begin{aligned} &f(\theta)\frac{\mathrm{d}^2\theta}{\mathrm{d}z^2} + \frac{k_{33}-k_{11}}{2}\sin(2\theta)\left(\frac{\mathrm{d}\theta}{\mathrm{d}z}\right)^2 \\ &+\frac{1}{2}\varepsilon_0\Delta\varepsilon\sin(2\theta)\left(\frac{\mathrm{d}\varphi}{\mathrm{d}z}\right)^2 + \frac{e_{11}+e_{33}}{2}\sin(2\theta)\frac{\mathrm{d}^2\varphi}{\mathrm{d}z^2} = 0, \end{aligned} \tag{7}$$

$$\begin{aligned} &\varepsilon_0\Delta\varepsilon\sin(2\theta)\left(\frac{\mathrm{d}\theta}{\mathrm{d}z}\right)\left(\frac{\mathrm{d}\varphi}{\mathrm{d}z}\right) \\ &+g(\theta)\left(\frac{\mathrm{d}^2\varphi}{\mathrm{d}z^2}\right) - (e_{11}+e_{33})\cos(2\theta)\left(\frac{\mathrm{d}\theta}{\mathrm{d}z}\right)^2 \\ &-\frac{1}{2}(e_{11}+e_{33})\sin(2\theta)\left(\frac{\mathrm{d}^2\theta}{\mathrm{d}z^2}\right) = 0. \end{aligned} \tag{8}$$

Equations (7) and (8) can be re-written as the following two equations for the strong anchoring boundary condition $\theta(0) = \theta(l) = 0$:

$$z = \begin{cases} Z, & 0 \le z \le l/2, \\ l - Z, & l/2 \le z \le l, \end{cases} \tag{9}$$

$$\begin{aligned} U &= \frac{1}{\varepsilon_0\varepsilon_\perp}\sqrt{\frac{1+\gamma\sin^2\theta_{\text{m}}}{\gamma}}\int_0^{\theta_{\text{m}}}\left[\frac{4\varepsilon_0\varepsilon_\perp k_{11}(1+\gamma\sin^2\theta)(1+\kappa\sin^2\theta)+(e_{11}+e_{33})^2\sin^2(2\theta)}{(\sin^2\theta_{\text{m}}-\sin^2\theta)(1+\gamma\sin^2\theta)^2}\right]^{1/2}\mathrm{d}\theta \\ &\quad -\frac{1}{\varepsilon_0\varepsilon_\perp}\int_0^{\theta_{\text{m}}}\frac{(e_{11}+e_{33})\sin(2\theta)}{1+\gamma\sin^2\theta}\mathrm{d}\theta, \end{aligned} \tag{10}$$

where

$$Z = \frac{l}{2}\frac{\displaystyle\int_0^{\theta}\left[\frac{4\varepsilon_0\varepsilon_\perp k_{11}(1+\gamma\sin^2\theta)(1+\kappa\sin^2\theta)+(e_{11}+e_{33})^2\sin^2(2\theta)}{\sin^2\theta_{\text{m}}-\sin^2\theta}\right]^{1/2}\mathrm{d}\theta}{\displaystyle\int_0^{\theta_{\text{m}}}\left[\frac{4\varepsilon_0\varepsilon_\perp k_{11}(1+\gamma\sin^2\theta)(1+\kappa\sin^2\theta)+(e_{11}+e_{33})^2\sin^2(2\theta)}{\sin^2\theta_{\text{m}}-\sin^2\theta}\right]^{1/2}\mathrm{d}\theta},$$

$\gamma = \varepsilon_\parallel/\varepsilon_\perp$, $\kappa = k_{33}/k_{11}$, and θ_{m} is the tilt angle of the director at the intermediate liquid crystal layer, that is, $\theta_{\text{m}} = \theta(l/2)$.

By introducing new quantities $\eta = \sin^2\theta_{\text{m}}$, $\sin\theta = \sin\theta_{\text{m}}\sin\alpha$, and $e_{11}+e_{33} = e$, equations (9) and (10) can be simplified, respectively, as

$$\frac{\mathrm{d}z}{\mathrm{d}\theta} = \begin{cases} \dfrac{l}{2B}\left[\dfrac{4\varepsilon_0\varepsilon_\perp k_{11}(1+\gamma\sin^2\theta)(1+\kappa\sin^2\theta)+e^2\sin^2(2\theta)}{\sin^2\theta_{\text{m}}-\sin^2\theta}\right]^{1/2}, & 0 \le z \le l/2, \\ l - \dfrac{l}{2B}\left[\dfrac{4\varepsilon_0\varepsilon_\perp k_{11}(1+\gamma\sin^2\theta)(1+\kappa\sin^2\theta)+e^2\sin^2(2\theta)}{\sin^2\theta_{\text{m}}-\sin^2\theta}\right]^{1/2}, & l/2 \le z \le l, \end{cases} \tag{11}$$

$$U = \frac{1}{\varepsilon_0\varepsilon_\perp}\int_0^{\pi/2}\left\{\sqrt{\frac{1+\gamma\eta}{\gamma}}\left[\frac{4\varepsilon_0\varepsilon_\perp k_{11}(1+\gamma\eta\sin^2\alpha)(1+\kappa\eta\sin^2\alpha)+4e^2\eta\sin^2\alpha(1-\eta\sin^2\alpha)}{(1+\gamma\eta\sin^2\alpha)^2(1-\eta\sin^2\alpha)}\right]^{1/2} - \frac{e\eta\sin(2\alpha)}{(1+\gamma\eta\sin^2\alpha)}\right\}\mathrm{d}\alpha, \tag{12}$$

where

$$B = \int_0^{\pi/2}\left[\frac{4\varepsilon_0\varepsilon_\perp k_{11}(1+\gamma\eta\sin^2\alpha)(1+\kappa\eta\sin^2\alpha)+4e^2\eta\sin^2\alpha(1-\eta\sin^2\alpha)}{1-\eta\sin^2\alpha}\right]^{1/2}\mathrm{d}\alpha.$$

The LC cell can be seen as infinitesimal series capacitors of capacitance $\mathrm{d}C$, thickness $\mathrm{d}z$, and area S, then $\mathrm{d}C = S\varepsilon(z)/\mathrm{d}z$, and the total capacitance C is

$$\frac{1}{C} = \frac{l}{C_0 B}\int_0^{\pi/2}\left[\frac{4\varepsilon_0\varepsilon_\perp k_{11}\left(1+\gamma\eta\sin^2\alpha\right)\left(1+\kappa\eta\sin^2\alpha\right)+4e^2\eta\sin^2\alpha\left(1-\eta\sin^2\alpha\right)}{\left(1+\gamma\eta\sin^2\alpha\right)^2\left(1-\eta\sin^2\alpha\right)}\right]^{1/2}\mathrm{d}\alpha, \tag{13}$$

where $C_0 = S\varepsilon_0\varepsilon_\perp/l$ is the capacitance corresponding to zero voltage. By introducing reduced capacitance $c = C/C_0$, equation (13) can be simplified as

$$c = B/B_1, \tag{14}$$

where

$$B_1 = \int_0^{\pi/2}\left[\frac{4\varepsilon_0\varepsilon_\perp k_{11}\left(1+\gamma\eta\sin^2\alpha\right)\left(1+\kappa\eta\sin^2\alpha\right)+4e^2\eta\sin^2\alpha\left(1-\eta\sin^2\alpha\right)}{\left(1+\gamma\eta\sin^2\alpha\right)^2\left(1-\eta\sin^2\alpha\right)}\right]^{1/2}\mathrm{d}\alpha.$$

2.2. HAN cell

The configuration of the HAN cell is similar to that of the PAN cell. Unlike the PAN cell, the lower substrate of the HAN cell is treated to induce a parallel strong anchoring of the director, whereas its upper substrate is treated to give a perpendicular strong anchoring. When an external voltage U perpendicular to the plane of the substrate with zero electric potential at the lower substrate is applied to the cell, the maximum tilt angle of the director is fixed on the upper substrate. In this case, the equilibrium equation is not changed, which remains to be Eqs. (7) and (8). The following deduction of the HAN cell is different from that of the PAN cell.

Without an applied voltage, the equation of the tilt angle with strong anchoring boundary conditions $\theta(0) = 0$ and $\theta(l) = \pi/2$ can be written as

$$z = l\frac{\displaystyle\int_0^{\theta}\left[1+\kappa\sin^2\theta+\frac{e^2}{4k_{11}\varepsilon_0\varepsilon_\perp}\frac{\sin^2(2\theta)}{1+\gamma\sin^2\theta}\right]^{1/2}\mathrm{d}\theta}{\displaystyle\int_0^{\pi/2}\left[1+\kappa\sin^2\theta+\frac{e^2}{4k_{11}\varepsilon_0\varepsilon_\perp}\frac{\sin^2(2\theta)}{1+\gamma\sin^2\theta}\right]^{1/2}\mathrm{d}\theta}. \tag{15}$$

With an applied voltage, the equations of the tilt angle and the potential can be re-written as

$$z = l\frac{\displaystyle\int_0^{\theta}\left(H+\frac{1}{1+\gamma\sin^2\theta}\right)^{-1/2}\left[1+\kappa\sin^2\theta+\frac{e^2}{4k_{11}\varepsilon_0\varepsilon_\perp}\frac{\sin^2(2\theta)}{1+\gamma\sin^2\theta}\right]^{1/2}\mathrm{d}\theta}{\displaystyle\int_0^{\pi/2}\left(H+\frac{1}{1+\gamma\sin^2\theta}\right)^{-1/2}\left[1+\kappa\sin^2\theta+\frac{e^2}{4k_{11}\varepsilon_0\varepsilon_\perp}\frac{\sin^2(2\theta)}{1+\gamma\sin^2\theta}\right]^{1/2}\mathrm{d}\theta}, \tag{16}$$

$$U = \int_0^{\pi/2}\left(\frac{k_{11}}{\varepsilon_0\varepsilon_\perp}\right)^{1/2}\left(1+\gamma\sin^2\theta\right)^{-1}\left(H+\frac{1}{1+\gamma\sin^2\theta}\right)^{-1/2}\left[1+\kappa\sin^2\theta+\frac{e^2}{4k_{11}\varepsilon_0\varepsilon_\perp}\frac{\sin^2(2\theta)}{1+\gamma\sin^2\theta}\right]^{1/2}\mathrm{d}\theta$$
$$-\int_0^{\pi/2}\frac{e}{\varepsilon_0\varepsilon_\perp}\frac{\sin(2\theta)}{1+\gamma\sin^2\theta}\mathrm{d}\theta, \tag{17}$$

where H is a constant that relates to the voltage.

According to the definition of the capacitor in the LC cell mentioned above, the expression of capacitance in the HAN cell for zero applied voltage is

$$c = M/M_1, \tag{18}$$

where

$$M = \int_0^{\pi/2}\left[k_{11}\left(1+\kappa\sin^2\theta\right)+\frac{e^2}{4\varepsilon_0\varepsilon_\perp}\frac{\sin^2(2\theta)}{1+\gamma\sin^2\theta}\right]^{1/2}\mathrm{d}\theta,$$

$$M_1 = \int_0^{\pi/2}\left[k_{11}\left(1+\kappa\sin^2\theta\right)+\frac{e^2}{4\varepsilon_0\varepsilon_\perp}\frac{\sin^2(2\theta)}{1+\gamma\sin^2\theta}\right]^{1/2}$$
$$\times\left(1+\gamma\sin^2\theta\right)^{-1}\mathrm{d}\theta.$$

The expression of capacitance in the HAN cell for an applied voltage can be written as

$$c = N/N_1, \tag{19}$$

where

$$N = \int_0^{\pi/2}\left(H+\frac{1}{1+\gamma\sin^2\theta}\right)^{-1/2}$$
$$\times\left[4k_{11}\varepsilon_0\varepsilon_\perp\left(1+\kappa\sin^2\theta\right)+\frac{e^2\sin^2(2\theta)}{1+\gamma\sin^2\theta}\right]^{1/2}\mathrm{d}\theta,$$

$$N_1 = \int_0^{\pi/2} \left(H + \frac{1}{1+\gamma\sin^2\theta}\right)^{-1/2} \times \left[4k_{11}\varepsilon_0\varepsilon_\perp\left(1+\kappa\sin^2\theta\right) + \frac{e^2\sin^2(2\theta)}{1+\gamma\sin^2\theta}\right]^{1/2} \times \left(1+\gamma\sin^2\theta\right)^{-1} \mathrm{d}\theta.$$

3. Numerical simulation

Based on the theoretical deduction, the c–U and c–e curves and the distributions of the director and the electric potential can be calculated numerically using Matlab. The concrete calculation for the PAN cell is as the follows. (i) When U and e are determinate, the value of η in the scope from 0 to 1 can be known from Eq. (12). (ii) By substituting η into Eq. (14), one can obtain the reduced capacitance c. If the flexoelectric coefficients are constant, then the c–U curve can be obtained. If the applied voltage is constant, then the c–e curve can be obtained. (iii) The distribution of the director can be readily obtained from Eq. (11) by replacing η with respect to different applied voltages and flexoelectric coefficients. (iv) Once the distribution of the director is determined, the distribution of the electric potential can also be obtained from Eq. (4). The concrete calculation for the HAN cell is analogue to that for the PAN cell. In calculations, the material parameters of the LC are shown in Table 1. The thickness of the LC cell is 4 μm. The sum of flexoelectric coefficients is limited in the interval from −50 pC/m to 50 pC/m due to the limit of the flexoelectric coefficients.[27] The c–U and c–e curves for the two cells are shown in Figs. 1 and 2. Figure 1(a) is very similar to Fig. 5 in Ref. [11], which shows that our simulation is reliable. While Brown and Mottram gave the permittivity–U curve, we give the reduced capacitance–U curve. In fact, the change of the permittivity can reflect the change of the capacitance.

Table 1. Material parameters of the LC.

k_{11}/pN	k_{33}/pN	$\varepsilon_\perp$	$\Delta\varepsilon$
6.2	8.3	5.3	5.2

From Figs. 1 and 2, we can see that the flexoeletric effect has different influences on the capacitances of the two kinds of LC cells for different flexoelectric coefficients and applied voltages. The dependence of the capacitance on the sum of flexoelectric coefficients in the PAN cell is symmetrical according to the case of ignoring the flexoelectric effect, and the larger the absolute value of e, the larger the difference of the capacitance. However, the dependence in the HAN cell is asymmetrical. The maximum capacitance in the HAN cell does not correspond to the case of the flexoelectric effect ignored, but exists in a certain position with positive flexoelectric coefficients. For the negative flexoelectric coefficients, the larger the absolute value of e, the larger the difference

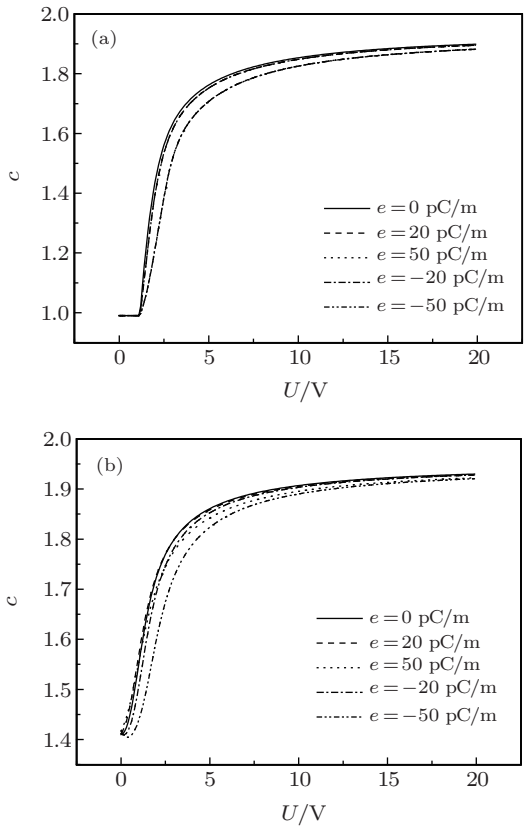


Fig. 1. The c–U curves of (a) PAN cell and (b) HAN cell.

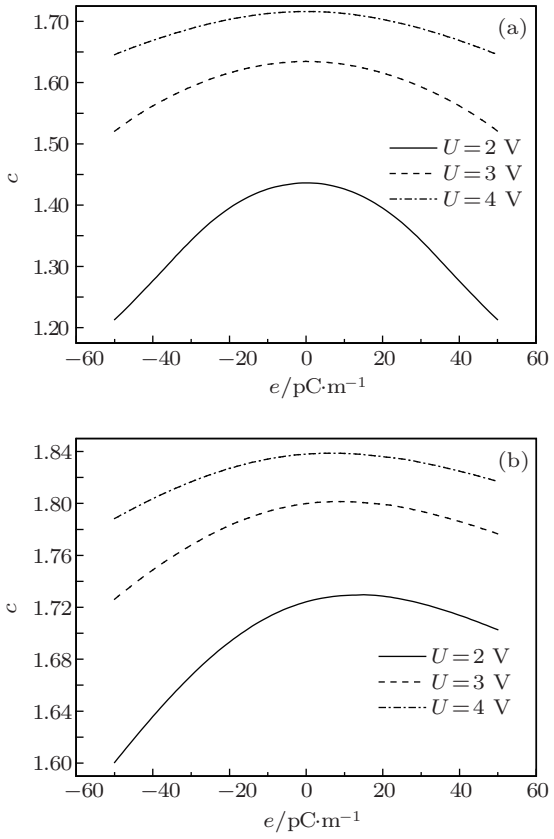


Fig. 2. The c–e curves of (a) PAN cell and (b) HAN cell.

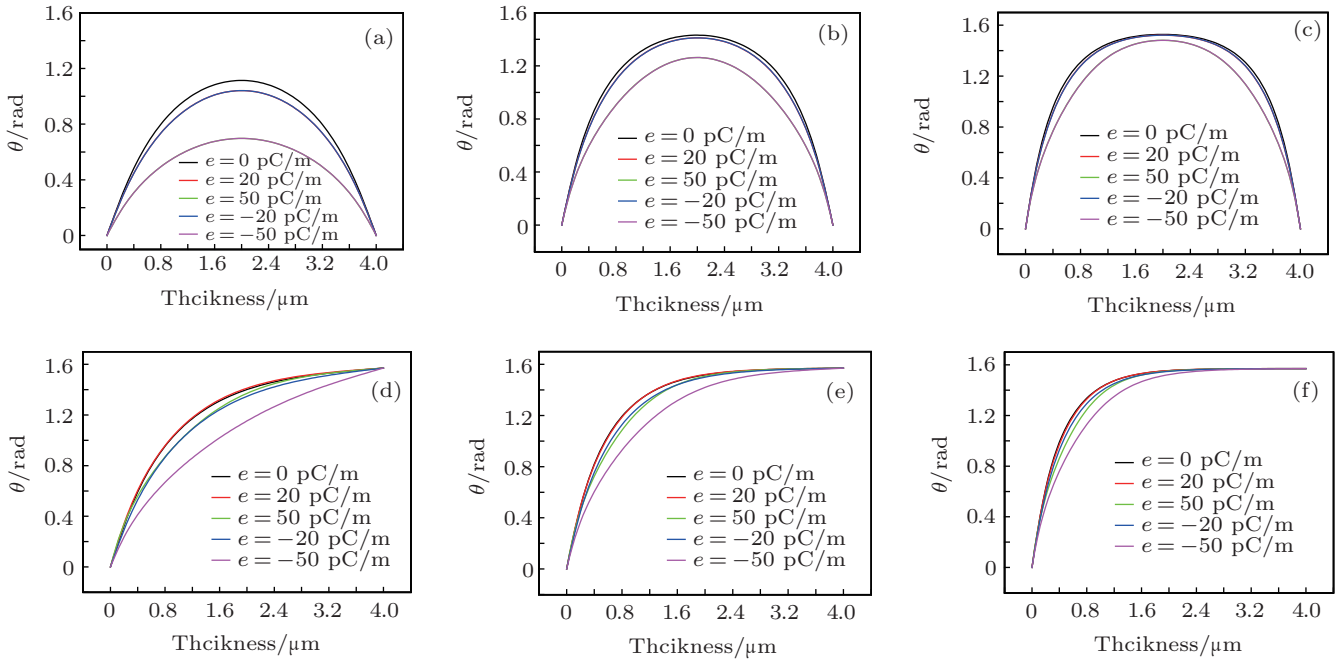


Fig. 3. (color online) Distributions of the director in (a)–(c) PAN cell and (d)–(f) HAN cell for different sums of flexoelectric coefficients.

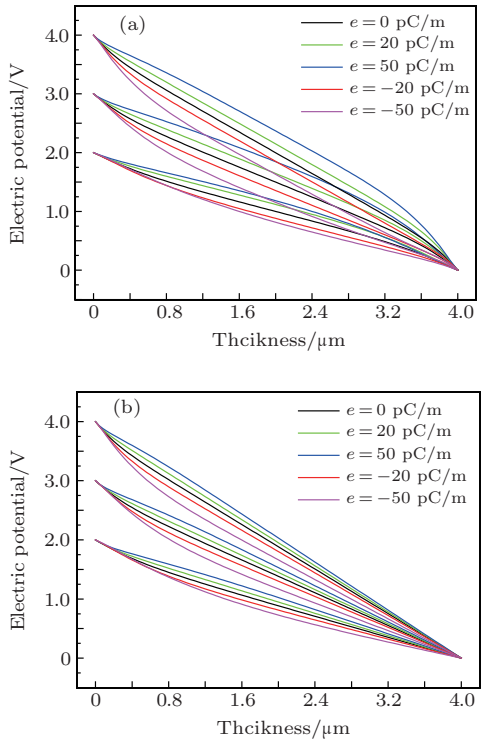


Fig. 4. (color online) Distributions of the electric potential in (a) PAN cell and (b) HAN cell for different sums of flexoelectric coefficients.

of the capacitance relative to the maximum. The changes of the c–U curve are quite small for the larger absolute value of e relative to no flexoelectric effect considered, as shown in Fig. 1, where the ordinate denotes the reduced capacitance. From the definition of the reduced capacitance, $c = C/C_0$, if the difference of the reduced capacitance is 0.01, then the actual deviation of the capacitance is 11.73 pF, with the assumption of $S = 10^{-4}$ m^2, which can be measured in experiment. These variations are in nature due to the reorientation of the liquid crystal molecules for different voltages. To illuminate this, we also calculate the distributions of the director and the electric potential for two kinds of LC cells, as shown in Figs. 3 and 4.

In the PAN cell, the distributions of the director with flexoelectric coefficients of different signs but of the same absolute value are uniform whether the external applied voltage is 2 V, 3 V, or 4 V, as seen in Figs. 3(a)–3(c). Figures 3(a)–3(c) are very similar to Fig. 4 in Ref. [11], which again shows that our simulation is reliable. However, the distributions of the director in the HAN cell for different flexoelectric coefficients and external applied voltages are very far apart from each other. There is always a difference for every external applied voltage, and the larger the external applied voltage, the smaller the difference, as seen in Figs. 3(d)–3(f). The main cause resulting in the reorientation of the liquid crystal molecules is the total electric field, including the induced internal field with the flexoelectric effect and the external applied field, which can be embodied by the electric potential. For the PAN cell, owing to the influence of the flexoelectric effect, the distributions of the electric potential with flexoelectric coefficients of different signs but of the same absolute value have a symmetry with respect to the distribution of ignoring the flexoelectric effect for every external applied voltage, as shown in Fig. 4(a). This kind of symmetry disappears in the HAN cell, as seen in Fig. 4(b).

These simulated results are very useful for us to determine the sum of flexoelectric coefficients by comparing them

with the experimental results. Once the absolute value of the sum of flexoelectric coefficients is determined, the sign of the sum of flexoelectric coefficients can be obtained by judging the monotonicity of the *c*–*U* curve. To avoid this case, the HAN cell in measuring is chosen and the external applied voltage should be as small as possible.

4. Experimental design for measuring the capacitance

The capacitance characteristics of the LC cell can usually be used to explore the dielectric constant and the elastic constant of the LC material. Owing to the influence of the flexoeletricity of the LC material on the capacitance characteristics of the LC cell, as shown in Fig. 2, the sum of flexoelectric coefficients can be determined by measuring the capacitance of the LC cell. In this section, we demonstrate the experimental design in detail.

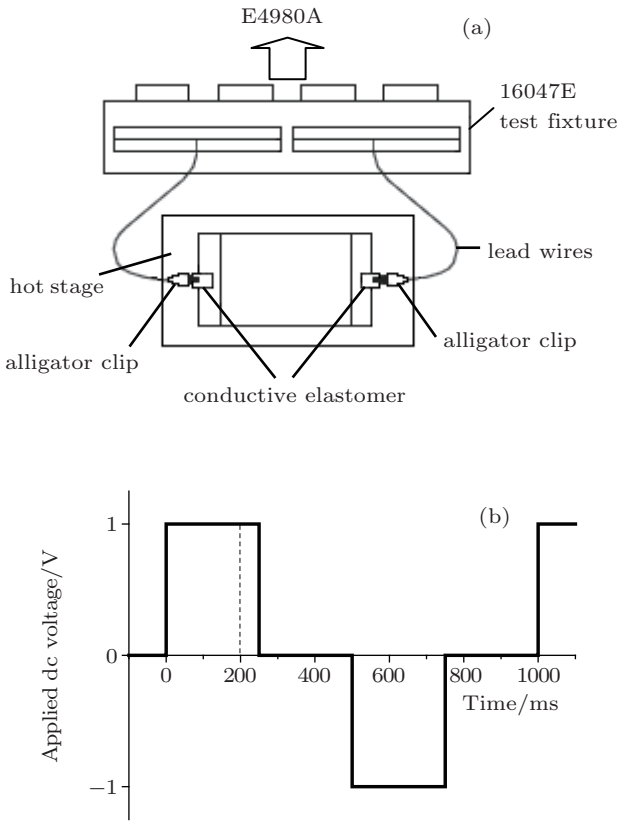


Fig. 5. (a) Experimental configuration for measuring the capacitance of LC cell and (b) the pulsed dc voltage signal.

In measuring the capacitance of the LC cell, an improved precision LCR meter E4980A (Agilent) is used and the LC cell is mounted on a hot stage (LTS350, Linkam) that is regulated by a hot controller (TP94, Linkam) to prevent the temperature influence on the capacitance. Unlike the usual precision LCR meter available in the market, the improved precision LCR meter E4980A (Agilent) can generate a pulsed dc voltage signal[35] as the test signal to measure the capacitance of the LC cell. The connection between the meter and the pulsed dc voltage signal are shown in Fig. 5. Two electrodes of the LC cell are held using two alligator clips and a conductive elastomer, with the lead wires connected to a test fixture 16047E. To eliminate the effects of the lead wires and the alligator clips connected to the test fixture, it is best to keep the length of the lead wires to a minimum. The aim of adopting the pulsed dc voltage signal is to prevent electrolytic decomposition of the liquid crystal and to minimize any effect of ion flow. Although a standard ac square wave can achieve this aim, the flexoelectric effect in this case will be ignored, as shown in Refs. [13] and [35]. When each positive pulsed dc voltage is applied to the LC cell, the capacitance is collected at the time of 200 ms to allow the director to reach equilibrium following the initial dynamic response of the cell.[36]

5. Discussion and conclusion

In the theoretical analysis we assume a pure insulating material filled in the LC cell. In fact, there are ions in any real system, which results in the ionic adsorption phenomenon to affect the capacitance. However, the density of the adsorptive ions is determined by cleaning techniques and time, as shown in Ref. [37]. A long time cleaning of the substrate can eliminate the influence of the adsorptive ions. As a result, we neglect the influence of ions in simulation and consider the LC as a pure insulating material.

In addition, in the numerical simulation, the elastic and dielectric constants of the LC material are seen as fixed values, and the flexoelectric coefficients are adjustable within the range from -50 pC/m to 50 pC/m, which contains the measurement value reported in the previous literature. If the elastic or dielectric constants have different values, then the result will definitely change, which can also be calculated using the above simulation method. Because a comparison between theory and experiment is not involved in this paper, the degeneracy of fitting parameters of the elastic constant k_{33} and the flexoelectric coefficient $e_{11}+e_{33}$, mentioned in Ref. [11], is not discussed in the current work. We will analyze the degeneracy in fitting the theoretical result to the measurements using the method introduced in Ref. [11] in a future publication.

In this paper, we analyze in detail the capacitance characteristics in strong anchoring PAN and HAN cells using the namatic continuum theory and calculate the dependence of the capacitance on both the flexoelectric coefficient and the voltage. The flexoelectric effect has a strong influence on the capacitances of the two cells. Therefore, we propose a method to determine the sum of flexoelectric coefficients by comparing the experimental data of the capacitance of the LC cell with the simulated value. We also present a feasible technique to measure the sum of flexoelectric coefficients.

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