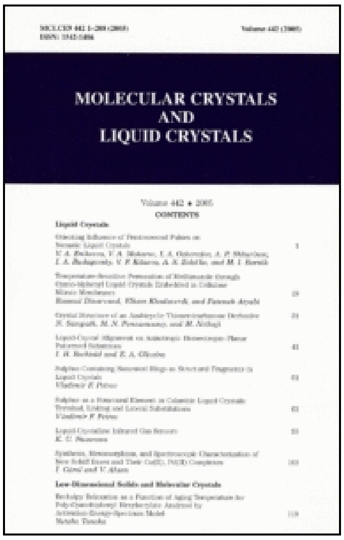
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Flexoelectric Effect in a HAN-IPS Cell

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Flexoelectric properties are evident in experiments preformed with hybrid aligned nematic. In this article, the flexoelectric effect in a hybrid aligned nematic in-plane switching liquid-crystal cell is investigated. The equations for the distribution of the liquid-crystal director and the expression of critical voltage in the one-constant approximation are obtained. The results of computer simulation show that the value of angle ϕ exceeds 90 degrees and closes to 180 degrees between the bottom substrate and the mid-layer.

Keywords Critical voltage; distribution of liquid crystal director; flexoelectric effect; hybrid aligned nematic; in-plane switching

Introduction

The properties of electric field–induced deformations of the director distribution in nematic liquid crystal (NLC) cell are twofold in nature: dielectric and flexoelectric. Flexoelectricity provides a reciprocal relationship between curvature distortions and electric polarization, which was described firstly by Robert Meyer in 1969 and later became known as the *flexoelectric effect* [1]. In the description of Meyer, the flexoelectric polarization should be proportional to the distortion:

$$\vec{p} = e_1(\nabla \cdot \vec{n})\vec{n} + e_3(\nabla \times \vec{n}) \times \vec{n}, \tag{1}$$

where e_1 and e_3 are the flexoelectric coefficients corresponding to splay and bend, respectively.

To date, flexoelectric coefficients of NLC have been measured mainly by analyzing optical effects produced by electric field induced director distortion [2]. In 2006, the giant bend flexoelectric coefficient was found in measuring the response of a bent-core liquid crystal using the electric current produced by periodic mechanical flexing of NLC's bounding surfaces [3], which has been reconfirmed by the converse flexoeffect [4]. But the later study of the converse flexoelectric effect in two other bent-core NLCs with opposite dielectric anisotropies revealed that the flexocoefficient was of the usual order of magnitude as in calamitics [5].

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The hybrid aligned nematic (HAN) cell is a type of liquid-crystal cell that has both splay and bend distortions in its initial state and flexoelectric properties are evident in experiments preformed with a HAN cell [2,3,6–14]. In liquid-crystal displays, several wide viewing angle and faster response time liquid-crystal modes such as in-plane switching (IPS) [15,16] and fringefield switching (FFS) [17–21] were developed previously. In this article, we investigate the flexoelectric effect in the hybrid aligned nematic in-plane switching (HAN-IPS) liquid-crystal mode on infinitely strong anchoring at both surfaces. The equations for the distribution of the liquid-crystal director and the expressions of critical voltage in the one-constant approximation are obtained using continuum theory and the numerical results show that compared with no flexoelectric effect, the value of angle ϕ exceeds 90 degrees and closes to 180 degrees between the bottom substrate and the mid-layer. The phenomenon can be not only evidence to prove the existence of the flexoelectric effect but also a method to obtain the floxelectric coefficient.

The Theory Description

The simplified model of the HAN-IPS is that supposing a uniform and in-plane switching electric field $E = \frac{U}{l}$ (l is the electrodes separated gap) applied to a HAN cell with two substrates at $x = -\frac{d}{2}$ and $x = \frac{d}{2}$ (d is liquid-crystal cell gap), respectively. The z axis is parallel to the direction of electric field. The anchoring at the boundaries is assumed to be strong. When the electric field is absent, the director in the plane of xy is described by angle ϕ. The z component of director induced by the external electric field can be described by introducing angle θ. The orientation of a liquid-crystal (LC) molecule can be characterized by the angle θ and angle ϕ, which is shown in Fig. 1. Then we have

$$\begin{aligned} \vec{n} &= (\cos\theta\cos\phi, \cos\theta\sin\phi, \sin\theta), \\ \vec{E} &= (0, 0, E), \end{aligned} \tag{2}$$

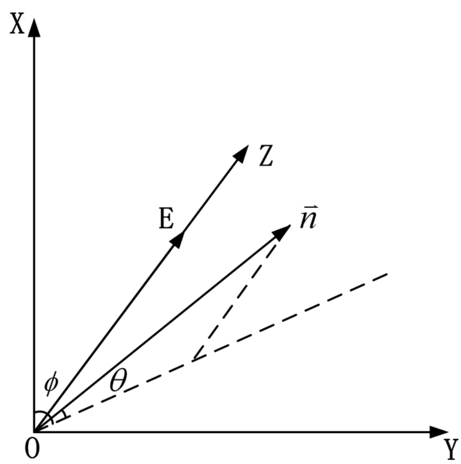

Figure 1. Spherical coordinate of molecular orientation.

and we assume that the distortion depends only on one dimension with $\theta = \theta(x)$, $\phi = \phi(x)$.

According to the elastic continuum theory, the Oseen-Frank strain free energy density is given by:

$$f_{el} = \frac{1}{2}K_{11}(\nabla \cdot \vec{n})^2 + \frac{1}{2}K_{22}(\vec{n} \cdot \nabla \times \vec{n})^2 + \frac{1}{2}K_{33}(\vec{n} \times \nabla \times \vec{n})^2, \tag{3}$$

where K_{11}, K_{22}, K_{33} are the elastic coefficients for splay, twist, and bend, respectively.

Exported to an external electric field $\vec{E}$, dielectric free energy density and the flexoelectric free energy density are given by:

$$f_d = -\frac{1}{2}\varepsilon_0[\varepsilon_\perp \vec{E}^2 + \Delta\varepsilon(\vec{E} \cdot \vec{n})^2], \tag{4}$$

$$f_p = -\vec{P} \cdot \vec{E}, \tag{5}$$

where $\Delta\varepsilon$ is the dielectric anisotropy. In the system, the total free energy density is the sum of elastic, dielectric, and flexoelectric contributions:

$$\begin{aligned} f &= f_{el} + f_d + f_p \\ &= \frac{1}{2}K_{11}\left[\sin^2\theta\cos^2\phi\left(\frac{d\theta}{dx}\right)^2 + \cos^2\theta\sin^2\phi\left(\frac{d\phi}{dx}\right)^2 \right. \\ &\quad \left. + 2\sin\theta\cos\theta\sin\phi\cos\phi\frac{d\theta}{dx}\frac{d\phi}{dx}\right] \\ &\quad + \frac{1}{2}K_{22}\left[\sin^2\phi\left(\frac{d\theta}{dx}\right)^2 + \sin^2\theta\cos^2\theta\cos^2\phi\left(\frac{d\phi}{dx}\right)^2 \right. \\ &\quad \left. - 2\sin\theta\cos\theta\sin\phi\cos\phi\frac{d\theta}{dx}\frac{d\phi}{dx}\right] \\ &\quad + \frac{1}{2}K_{33}\left[\cos^2\theta\cos^2\phi\left(\frac{d\theta}{dx}\right)^2 + \cos^4\theta\cos^2\phi\left(\frac{d\phi}{dx}\right)^2\right] \\ &\quad - \frac{1}{2}\varepsilon_0(\varepsilon_\perp + \Delta\varepsilon\sin^2\theta)\frac{U^2}{l^2} \\ &\quad + \left[(e_1\sin^2\theta - e_3\cos^2\theta)\cos\phi\frac{d\theta}{dx} + e_1\sin\theta\cos\theta\sin\phi\frac{d\phi}{dx}\right]\frac{U}{l}, \end{aligned} \tag{6}$$

The equilibrium configuration for the LC deformation profile under a given applied field is such that the total free energy has a minimal value subject to the boundary conditions. The Euler-Lagrange equations are given by [22]:

$$\frac{\partial f}{\partial \theta} - \frac{d}{dx}\left[\frac{\partial f}{\partial(d\theta/dx)}\right] = 0, \tag{7}$$

$$\frac{\partial f}{\partial \phi} - \frac{d}{dx}\left[\frac{\partial f}{\partial(d\phi/dx)}\right] = 0. \tag{8}$$

Inserting Eq. (6) into the Euler-Lagrange Eq. (7) and Eq. (8), the equations for the distribution of liquid crystal director can be written as:

$$
\begin{aligned}
&(K_{11}-K_{33})\sin\theta\cos\theta\cos^2\phi\left(\frac{d\theta}{dx}\right)^2+[2(K_{33}-K_{22})\cos^2\theta\cos^2\phi+K_{11}\cos^2\phi \\
&\quad+K_{22}\sin^2\phi]\sin\theta\cos\theta\left(\frac{d\phi}{dx}\right)^2+(K_{11}\sin^2\theta\cos^2\phi+K_{22}\sin^2\phi+K_{33}\cos^2\theta\cos^2\phi) \\
&\quad\times\frac{d^2\theta}{dx^2}+\left(K_{11}-K_{22}\right)\sin\theta\cos\theta\sin\phi\cos\phi\frac{d^2\phi}{dx^2}+2(K_{22}-K_{11}\sin^2\theta-K_{33}\cos^2\theta) \\
&\quad\times\sin\phi\cos\phi\frac{d\theta}{dx}\frac{d\phi}{dx}+\varepsilon_0\Delta\varepsilon\sin\theta\cos\theta\left(\frac{U}{l}\right)^2-(e_1-e_3)\cos^2\theta\sin\phi\frac{d\phi}{dx}\frac{U}{l}=0,
\end{aligned}
\tag{9}
$$

and

$$
\begin{aligned}
&(K_{11}+K_{33}-2K_{22})\cos^2\theta\sin\phi\cos\phi\left(\frac{d\theta}{dx}\right)^2+(K_{11}-K_{22}\sin^2\theta-K_{33}\cos^2\theta) \\
&\quad\times\cos^2\theta\sin\phi\cos\phi(\frac{d\phi}{dx})^2+(K_{11}-K_{22})\sin\theta\cos\theta\sin\phi\cos\phi\frac{d^2\theta}{dx^2} \\
&\quad+(K_{11}\sin^2\phi+K_{22}\sin^2\theta\cos^2\phi+K_{33}\cos^2\theta\cos^2\phi)\cos^2\theta\frac{d^2\phi}{dx^2} \\
&\quad+2[K_{22}(\cos^2\theta-\sin^2\theta)\cos^2\phi-K_{11}\sin^2\phi-2K_{33}\cos^2\theta\cos^2\phi]\sin\theta\cos\theta\frac{d\theta}{dx}\frac{d\phi}{dx} \\
&\quad+(e_1-e_3)\cos^2\theta\sin\phi\frac{d\theta}{dx}\frac{U}{l}=0
\end{aligned}
\tag{10}
$$

In the one-constant approximation ($K=K_{11}=K_{22}=K_{33}$), the total free energy density and the equations for the distribution of liquid-crystal director are reduced to:

$$
\begin{aligned}
f&=f_{el}+f_d+f_p \\
&=\frac{1}{2}K\left[\left(\frac{d\theta}{dx}\right)^2+\cos^2\theta\left(\frac{d\phi}{dx}\right)^2\right]-\frac{1}{2}\varepsilon_0(\varepsilon_\perp+\Delta\varepsilon\sin^2\theta)\frac{U^2}{l^2} \\
&\quad+\left[(e_1\sin^2\theta-e_3\cos^2\theta)\cos\phi\frac{d\theta}{dx}+e_1\sin\theta\cos\theta\sin\phi\frac{d\phi}{dx}\right]\frac{U}{l}
\end{aligned}
\tag{11}
$$

$$
K\sin\theta\cos\theta\left(\frac{d\phi}{dx}\right)^2+K\frac{d^2\theta}{dx^2}+\varepsilon_0\Delta\varepsilon\sin\theta\cos\theta\left(\frac{U}{l}\right)^2-(e_1-e_3)\cos^2\theta\sin\phi\frac{d\phi}{dx}\frac{U}{l}=0
\tag{12}
$$

and

$$
K\cos\theta\frac{d^2\phi}{dx^2}-2K\sin\theta\frac{d\theta}{dx}\frac{d\phi}{dx}+(e_1-e_3)\cos\theta\sin\phi\frac{d\theta}{dx}\frac{U}{l}=0.
\tag{13}
$$

The boundary conditions of strong planar anchoring at the surfaces can be written as:

$$\theta\left(-\frac{d}{2}\right) = 0, \quad \theta\left(\frac{d}{2}\right) = 0,$$
$$\phi\left(-\frac{d}{2}\right) = \Phi, \quad \phi\left(\frac{d}{2}\right) = 0, \tag{14}$$

where Φ is the different value of angle ϕ between top and bottom substrates.

By the method of Derfel [23], small deformations of its distribution are assumed and the twist angle θ and tilt angle ϕ can be approximated respectively by their first Fourier series

$$\theta(x) = \xi\cos\left(\frac{\pi x}{d}\right),$$
$$\phi(x) = \frac{\Phi}{2} - \frac{\Phi}{d}x + \chi\sin\left(\frac{2\pi x}{d}\right), \tag{15}$$

where ξ and χ are small parameters.

Then Eq. (11) can be written as

$$\begin{aligned} f = &\frac{1}{2}K\left\{\xi^2\sin^2\left(\frac{\pi x}{d}\right)\frac{\pi^2}{d^2} + \cos^2\left[\xi\cos\left(\frac{\pi x}{d}\right)\right]\left[-\frac{\Phi}{d} + \chi\cos\left(\frac{2\pi x}{d}\right)\frac{2\pi}{d}\right]^2\right\} \\ &- \frac{1}{2}\frac{U^2}{l^2}\varepsilon_0\left\{\varepsilon_\perp + \Delta\varepsilon\sin^2\left[\xi\cos\left(\frac{\pi x}{d}\right)\right]\right\} - \left(\left[e_1\sin^2\left[\xi\cos\left(\frac{\pi x}{d}\right)\right]\right.\right. \\ &\left. - e_3\cos^2\left[\xi\cos\left(\frac{\pi x}{d}\right)\right]\right]\cos\left[\frac{\Phi}{2} - \frac{\Phi}{d}x + \chi\sin\left(\frac{2\pi x}{d}\right)\right] \\ &\times \xi\sin\left(\frac{\pi x}{d}\right)\frac{\pi}{d} + e_1\sin\left[\xi\cos\left(\frac{\pi x}{d}\right)\right]\cos\left[\xi\cos\left(\frac{\pi x}{d}\right)\right] \\ &\left.\times \sin\left[\frac{\Phi}{2} - \frac{\Phi}{d}x + \chi\sin\left(\frac{2\pi x}{d}\right)\right]\left[-\frac{\Phi}{d} + \chi\cos\left(\frac{2\pi x}{d}\right)\frac{2\pi}{d}\right]\right)\frac{U}{l} \end{aligned} \tag{16}$$

At $\xi = 0$, $\chi = 0$, the second derivative matrix is given by

$$F_{\xi,\xi}(0,0) = \int_{-\frac{d}{2}}^{\frac{d}{2}} f_{\xi,\xi}(0,0)dx = \frac{1}{2}\left(K\frac{\pi^2}{d} - K\frac{\Phi^2}{d} - \varepsilon_0\Delta\varepsilon d\frac{U^2}{l^2}\right), \tag{17}$$

$$F_{\xi,\chi}(0,0) = F_{\chi,\xi}(0,0) = \int_{-\frac{d}{2}}^{\frac{d}{2}} f_{\xi,\chi}(0,0)dx = \frac{2\pi^2(e_1 - e_3)(3\pi^2 - \Phi^2)}{(9\pi^2 - \Phi^2)(\pi^2 - \Phi^2)}\sin\Phi\frac{U}{l}, \tag{18}$$

$$F_{\chi,\chi}(0,0) = \int_{-\frac{d}{2}}^{\frac{d}{2}} f_{\chi,\chi}(0,0)dx = \frac{2\pi^2 K}{d}. \tag{19}$$

Using the condition

$$\det[F_{\xi,\xi}(0,0); F_{\xi,\chi}(0,0); F_{\chi,\xi}(0,0); F_{\chi,\chi}(0,0)] = 0, \tag{20}$$

the critical voltage is given by the following expression

$$U_c = \frac{Kl}{d}\left\{\frac{\pi^2 - \Phi^2}{\varepsilon_0 \Delta\varepsilon K + \left[\frac{2\pi \sin\Phi(e_1 - e_3)(3\pi^2 - \Phi^2)}{(9\pi^2 - \Phi^2)(\pi^2 - \Phi^2)}\right]^2}\right\}^{1/2}. \quad (21)$$

When $\Phi = \pi/2$, Eq. (21) reduces to

$$U_c = \frac{Kl}{d}\left\{\frac{3\pi^2/4}{\varepsilon_0 \Delta\varepsilon K + \left[\frac{88(e_1 - e_3)}{105\pi}\right]^2}\right\}^{1/2}, \quad (22)$$

where the term of $\left[\frac{88(e_1-e_3)}{105\pi}\right]^2$ is caused by flexoelectric effect decrease critical voltage.

Therefore, we find that the critical voltage is smaller with flexoelectric effect than not.

Numerical Results

A cell was filled with the 5CB, with the following 5CB liquid-crystal parameters employed:

$$K_{11} = 5.85 \times 10^{-12} N, \quad K_{22} = 3.0 \times 10^{-12} N, \quad K_{33} = 7.8 \times 10^{-12} N, \quad \Delta\varepsilon = 8.2,$$
$$d = 6.0 \times 10^{-6} m, \quad l = 9.0 \times 10^{-6} m, \quad e_1 - e_3 = 1.5 \times 10^{-11}\, C/m, \quad \Phi = \frac{\pi}{2}.$$

The director distribution is determined by finding the solution of Eq. (9) and Eq. (10) in an iterative numerical method. When the pretilt is 1 degree, the calculated

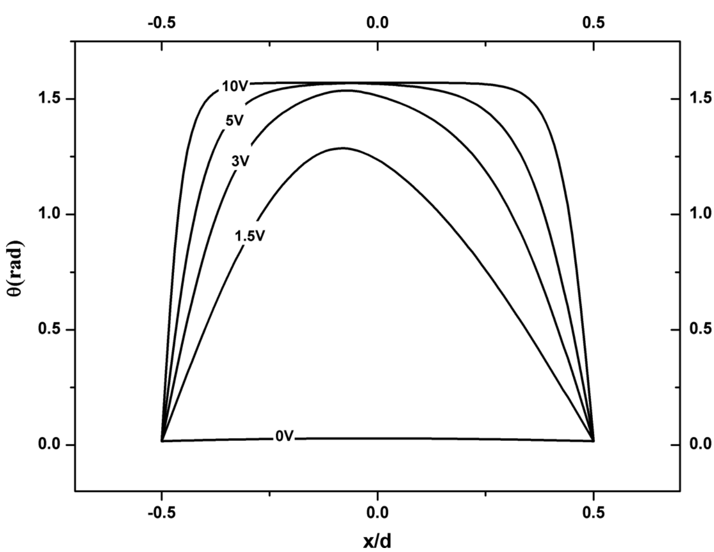

Figure 2. Variety of angle θ versus x/d under different voltage without the flexoelectric effect.

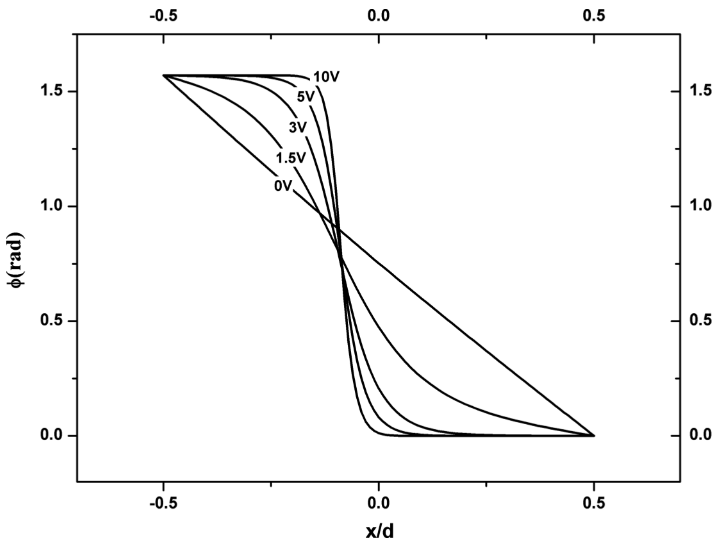

Figure 3. Variety of angle ϕ versus x/d under different voltage without the flexoelectric effect.

profiles for the angle θ and angle ϕ under different U are shown as functions of the nondimensional parameter x/d in Figs. 2 to 5. In the one-constant approximation $K = (K_{11} + K_{22} + K_{33})/3 = 5.55 \times 10^{-12} N$, the angle ϕ under different U is shown as a function of the nondimensional parameter x/d without and with flexoelectric effect in Figs. 6 and 7.

Figure 2 and 3 describe the angle θ and angle ϕ, respectively, under different voltages 0, 1.5, 3.0, 5.0, and 10.0 V without the flexoelectric effect, and profiles of the two angles considering the flexoelectric effect are drawn in Figs. 4 and 5. Comparing

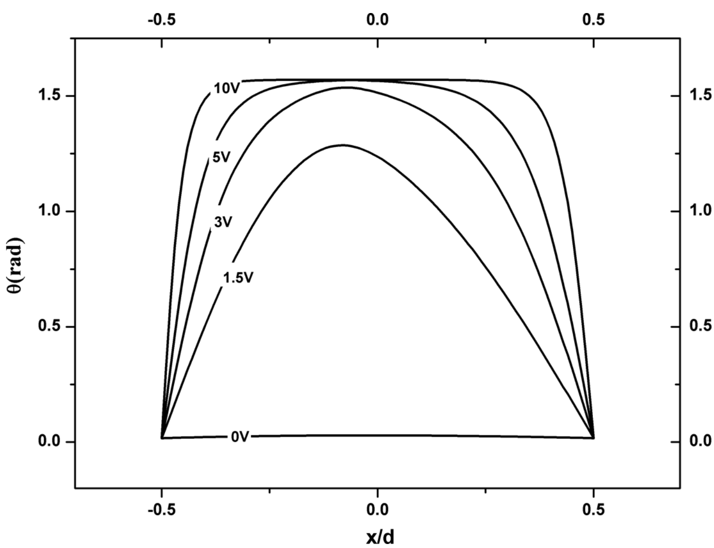

Figure 4. Variety of angle θ versus x/d under different voltage with the flexoelectric effect.

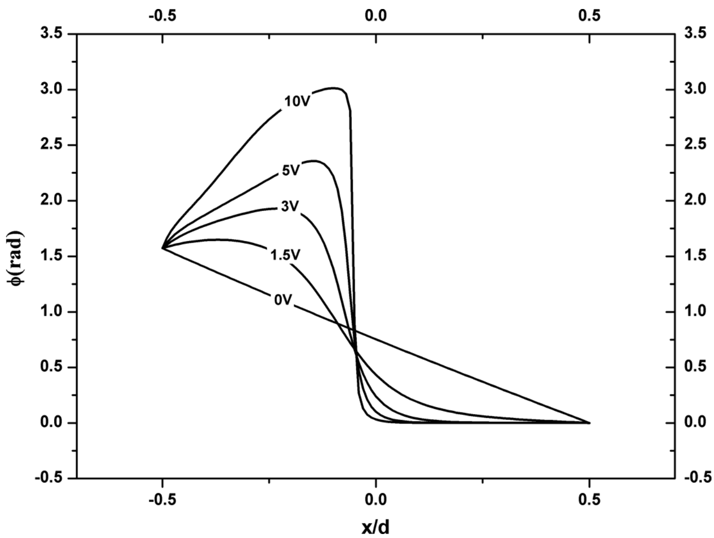

Figure 5. Variety of angle ϕ versus x/d under different voltage with the flexoelectric effect.

Fig. 3 with Fig. 5, we find that the angle ϕ in Fig. 5 is between 90 and 180 degrees in the bottom substrate and the mid-layer. Apply enough voltage to the HAN cell, the align mode of LC molecular in cell is shown in Fig. 8. In a numerical calculation, we find that the distribution of the LC director cannot be described by one dimension $\theta = \theta(x)$ and $\phi = \phi(x)$ if the value of $e_1 - e_3$ exceeds the order of magnitude of 10^{-11} C/m. Therefore, the giant flexoelectric coefficients should lead to some new director configuration.

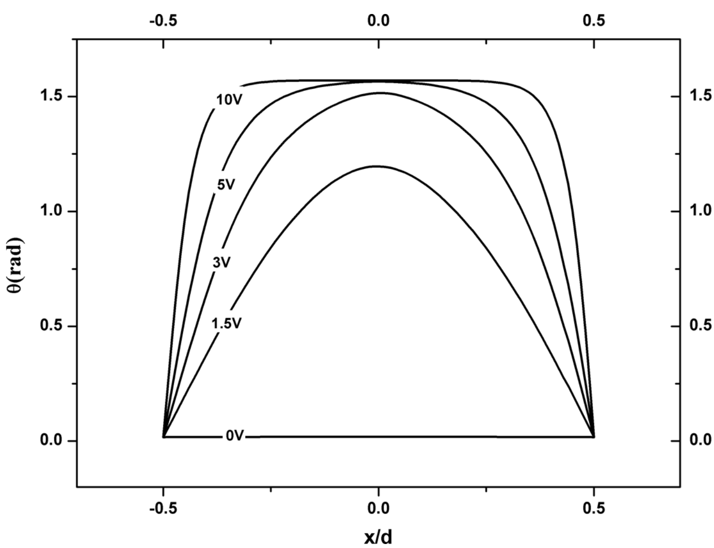

Figure 6. Variety of angle ϕ versus x/d under different voltage without the flexoelectric effect in the one-constant approximation.

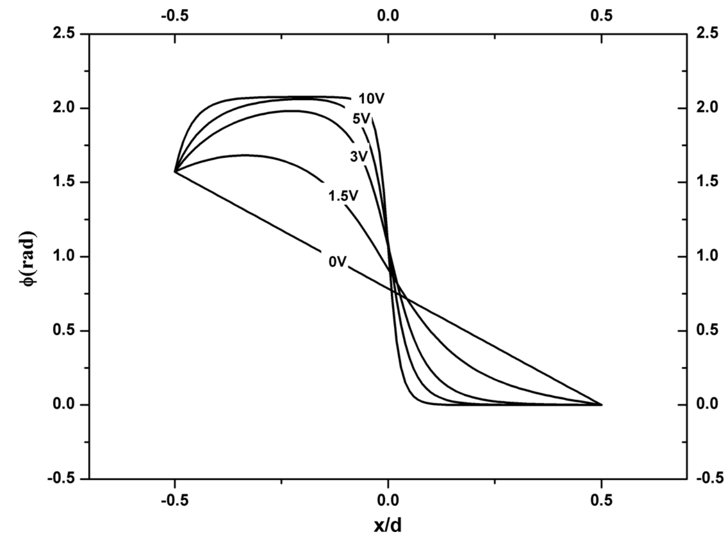

Figure 7. Variety of angle ϕ versus x/d under different voltage with the flexoelectric effect in the one-constant approximation.

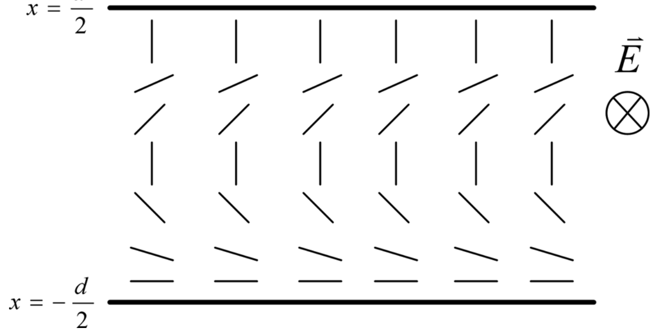

Figure 8. The align mode of liquid-crystal molecule in *x*y plane of a cell after enough voltage.

Due to the influence of the flexoelectric effect in the HAN-IPS, the flexoelectric coefficient $e_1 - e_3$ found by experiment can be tested using the method. The angle ϕ close to 180 degrees is caused by just the flexoelectric coefficient $e_1 - e_3$. Contrarily, if the distribution of the LC director is obtained in certain method, that is, wave-guide-mode technique, the flexoelectric coefficient $e_1 - e_3$ can be obtained using Eq. (9) and Eq. (10) in a HAN-IPS cell.

Conclusion

We have successfully investigated the flexoelectric effect in a HAN-IPS cell using a simple model. The distribution of the LC director and the critical voltage in the one-constant approximation of a HAN-IPS cell with the flexoelectric effect are obtained. The expression of critical voltage has never been reported as for as we know. The numerical results show that compared with no flexoelectric effect, the value of angle ϕ is between 90 and 180 degrees in the bottom substrate and the mid-layer (see Figs. 5 and 7) with the flexoelectric effect in a system. So it is necessary to consider the flexoelectric effect in most practical cases because the quality of the display effect of LCD mostly lies with the distribution of the LC director. Moreover, we introduce a potential method to test or to obtain the value of the flexoelectric coefficient $e_1 - e_3$.

Acknowledgment

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