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Computer modelling of the director configuration in a supertwist nematic liquid crystal cell

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The director distribution in a supertwist nematic cell, containing La-Roche liquid crystal mixture 3010, has been studied extensively using Berreman's computer simulation approach. It is seen that the director distribution in the cell depends critically on the total twist angle ϕ_t, the surface tilt angle θ_0 and the ratio of the cell thickness to the pitch d/p. The values of θ_0 and ϕ_t have been optimized to yield a small bistability ($\Delta V = 0{\cdot}06\,V$) and a relatively large change in the midplane tilt angle ($\Delta\theta_m = 51°$) in an unstrained cell with $\phi_t = (d/p) \times 360°$. The optimum values of θ_0 and ϕ_t were found to be 15° and 240°, respectively. The effect of varying d/p on the director distribution has also been studied in great detail in supertwist cells with $\theta_0 = 30°$ and $\phi_t = 270°$. Some interesting features in understrained and overstrained cells have been observed.

1. Introduction

New electro-optic effects with extremely sharp transmission characteristics have recently been reported in highly twisted nematic liquid crystal cells which have also been termed as (*a*) supertwist nematic (STN) [1], supertwist birefringent effect (SBE) [2] and (*b*) optical mode interference (OMI) [3] displays according to the choice of material and device parameters. These displays exhibit a small bistability, wider viewing angle and better contrast than the conventional twist nematic displays. They offer great potential for the development of complex high information content displays. Computer modelling of these supertwist cells would greatly help in elucidating the role of the various material and device parameters on their performance characteristics.

We report here the results of our numerical computations of the director distribution in a supertwist nematic cell containing La-Roche mixture 3010 following Berreman's approach [4]. It is seen that the director distribution depends critically on the total twist angle, ϕ_t, the surface tilt angle, θ_0, and the ratio of cell thickness to pitch, d/p. The angles ϕ_t and θ_0 have been optimized to yield a very small bistability ($\Delta V = 0{\cdot}06\,V$) and a relatively large change in the midplane tilt angle ($\Delta\theta_m = 51°$) for an unstrained cell. The effect of varying d/p has also been studied in great detail for high tilted (270°) cells. Some interesting features have been observed in understrained and overstrained cells.

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2. Theory

The strain free energy density of a chiral nematic liquid crystal is given by the Frank continuum equation [5]

$$F_s = \tfrac{1}{2}K_{11}(\nabla\cdot\mathbf{n})^2 + \tfrac{1}{2}K_{22}(\mathbf{n}\cdot\nabla\times\mathbf{n} - 2\pi/p)^2 + \tfrac{1}{2}K_{33}(\mathbf{n}\times\nabla\times\mathbf{n})^2, \tag{1}$$

where the symbols have their usual meaning. The director orientation at any point in the cell is characterized by the tilt angle θ and the twist angle ϕ with the components of the director $\mathbf{n}$ along the three principal axes being

$$\begin{aligned} n_z &= \sin\theta, \\ n_y &= \cos\theta\sin\phi, \\ n_x &= \cos\theta\cos\phi. \end{aligned}$$

The surface free energy per unit surface area can then be expressed as

$$F_s = \tfrac{1}{2}K_{11}(\theta'\cos\theta)^2 + \tfrac{1}{2}K_{22}(\phi'\cos^2\theta - 2\pi/p)^2 + \tfrac{1}{2}K_{33}\sin^2\theta[\theta'^2 + (\phi'\cos\theta)^2], \tag{2}$$

where

$$\theta' = \frac{d\theta}{dz}, \qquad \phi' = \frac{d\phi}{\partial z}$$

If an external voltage, V, is applied to the cell, the electrostatic free energy density will be

$$F_e = D^2/2\varepsilon_0(\varepsilon_\parallel\sin^2\theta + \varepsilon_\perp\cos^2\theta). \tag{3}$$

For the equilibrium configuration the integral of the Helmholtz free energy density $F_h = F_e + F_s$ should have an extremum value subject to the conditions imposed at the boundaries. On applying the calculus of variation and after rearranging the terms, we obtain the non-linear differential equations [6]

$$\theta'' = \frac{\cos\theta\sin\theta}{K_{11}\cos^2\theta + K_{33}\sin^2\theta}(A + B + C + E), \tag{4}$$

where

$$\left.\begin{aligned} A &= (K_{33} - K_{11})\theta'^2 \\ B &= 2K_{22}\phi'(\phi'\cos^2\theta - 2\pi/p), \\ C &= K_{33}\phi'^2(\sin^2\theta - \cos^2\theta), \\ E &= \frac{D^2(\varepsilon_\parallel - \varepsilon_\perp)}{\varepsilon_0(\varepsilon_\parallel\sin^2\theta + \varepsilon_\perp\cos^2\theta)^2} \qquad D = \frac{V}{d}\varepsilon_0(\varepsilon_\parallel\sin^2\theta + \varepsilon_\perp\cos^2\theta), \\ \phi' &= \frac{(T/\cos^2\theta + K_{22}2\pi/p)}{K_{22}\cos^2\theta + K_{33}\sin^2\theta}, \end{aligned}\right\} \tag{5}$$

with T as the constant of integration. In the present case, the cell is assumed to be symmetric with the tilt angle $\theta = \theta_0$ at both the surfaces and the director angle in the middle of the cell has an extreme value with $\theta' = 0$. The twist angle in the middle is half of the total twist angle and the director orientation in the two halves is symmetric. We start integrating equations (4) and (5) from the middle layer by making estimates of θ and ϕ' and the integration is carried to the end of the cell. The values of θ and

ϕ so determined at the boundary must be consistent with the boundary conditions. Repeated estimation of θ and ϕ' at the middle layer is done until the desired tilt and twist angle at the boundary are obtained. As a model calculation the program has been tested to yield the uniform tilt configuration at the numerical threshold voltage and the error in solution for θ_0 and ϕ has been confined to a reasonable tolerance of about 0·1°.

3. Results and discussion

3.1. *General*

The director orientation, i.e. the tilt and the twist angle in a supertwist cell has been determined as a function of the applied voltage by solving equations (3) and (4) using the Runge–Kutta–Nyström method [6]. All of the computations have been made by chiral liquid crystal mixture 3010 with $K_{11} = 14{\cdot}4 \times 10^{-12}$ N, $K_{22} = 7{\cdot}0 \times 10^{-12}$ N, $K_{33} = 20{\cdot}02 \times 10^{-12}$ N and $\Delta\varepsilon = 8{\cdot}3$.

The threshold voltage in the present case has been defined as that at which the tilt angle is constant throughout the cell and is equal to the surface tilt angle θ_0 with $\theta' = 0$ and $\phi' = \phi_t/d$. Using these definitions, equation (4) can be solved to give

$$V_{\mathrm{th}} = \left(\frac{4\pi K_{22}(d/p) - K_{33}\phi_t + 2(K_{33} - K_{22})\phi_t^2 \cos^2\theta_0}{\Delta\varepsilon\,\varepsilon_0}\right)^{1/2}. \tag{6}$$

Since the optical transmission characteristics are mainly governed by the director orientation in the midplane, it was imperative to study the variation of the midplane tilt angle θ_m versus the applied voltage. Figure 1 shows the variation of θ_m in a supertwist cell with $\phi_t = 270°$; $d/p = 0{\cdot}75$ and $\theta_0 = 30°$. This figure apart from showing a rapid change in θ_m just above the threshold voltage also shows a finite bistability ΔV. It has been found that the threshold voltage V_{th}, the bistability ΔV and the change in the midplane tilt angle $\Delta\theta_m$ where

$$\Delta\theta_m = \theta_m(V_{\mathrm{th}} + 0{\cdot}05\,V) - \theta_m(V_{\mathrm{th}})$$

depends critically on the various device parameters, namely ϕ_t, θ_0 and d/p.

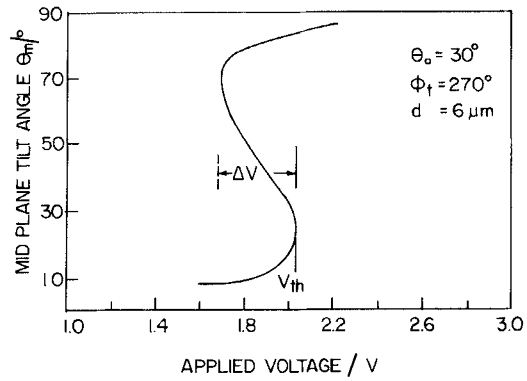

Figure 1. Variation of the midplane tilt angle θ_m with the applied voltage in a supertwist cell with $\phi_t = 270°$, $\theta_0 = 30°$ and $d/p = 0{\cdot}75$.

3.2. *Influence of the total twist angle* ϕ_t

The effect of ϕ_t on the director distribution has been computed by varying pitch so as to have $\phi_t = (d/p) \times 360°$ (that is the case of the unstrained pitch) with all other cell and material parameters remaining the same. Figure 2 shows the variation in the threshold voltage, bistability and change in the midplane tilt angle $\Delta\theta_m$ with increasing twist angle ϕ_t. It is seen that in the twist cells with $\phi_t < 180°$ the change in θ_m with applied voltage is extremely small and the bistability is zero. However, with increasing ϕ_t with $\phi_t > 180°$, θ_m shows a steeper variation with applied voltage and bistability also sets in. It is clearly seen from figure 2 that the bistability ΔV, the change in the midplane tilt angle $\Delta\theta_m$ and the threshold voltage V_{th} increases with increasing ϕ_t. As such the bistability increases from 0 to 0·55 V; $\Delta\theta_m$ increases from 6° to 58°, and V_{th} increases from 1·347 to 2·121 V as ϕ_t changes from 180° to 290°. It is quite evident that the twist angle ϕ_t plays an important role in enhancing the change in the midplane tilt angle which should greatly influence the contrast of the device. However, ϕ_t has to be optimized to obtain a sharp threshold and a small bistability.

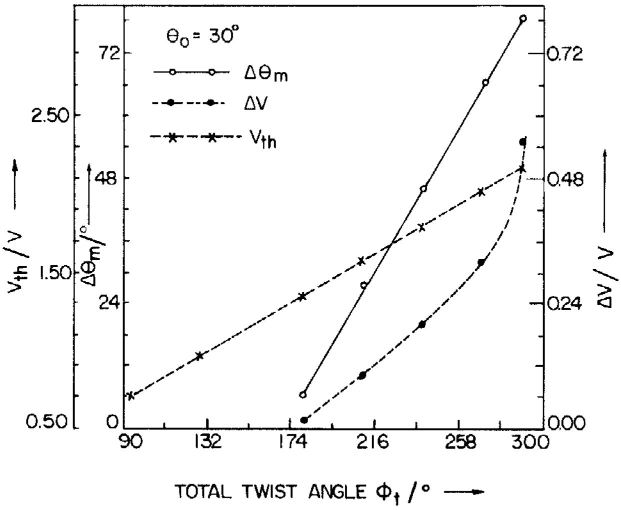

Figure 2. Variation of V_{th}, $\Delta\theta_m$ and ΔV with the total twist angle ϕ_t in a supertwist cell with $\theta_0 = 30°$ and $p = (d/\phi_t) \times 360°$.

3.3. *Influence of the surface tilt angle* θ_0

The surface tilt angle θ_0 also affects the performance characteristics of a supertwist cell critically. We have computed the effect of θ_0 on the director distribution in a 270° device, keeping all other material and device parameters the same. Figure 3 shows the variation in the bistability ΔV, the change in the midplane tilt angle $\Delta\theta_m$ and the threshold voltage V_{th} with the surface tilt angle θ_0. It is seen immediately that the bistability increases from 0·03 to 0·32 V when the surface tilt angle increases from 0° to 30°. However, the threshold sharpness, i.e. the change in midplane tilt angle $\Delta\theta_m$, decreases with increasing surface tilt angle and as such $\Delta\theta_m$ for a 0° surface tilt angle cell decreases from 72° to 55° for a 30° surface tilt angle cell. Similarly the threshold voltage also decreases with increasing surface tilt angle as calculated from equation (6). It is clear from this analysis that a supertwist cell with a lower surface tilt angle should have a better performance characteristic than a larger surface tilt cell.

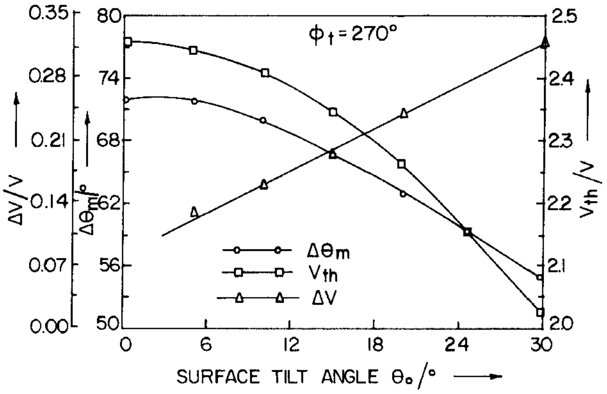

Figure 3. Variation of V_{th}, $\Delta\theta_m$ and ΔV with the surface tilt angle θ_0 in a supertwist cell with $\phi_t = 270°$ and $d/p = 0{\cdot}75$.

3.4. *Optimization of the surface tilt and total twist angles*

These results demonstrate quite vividly that the cell parameters ϕ_t and θ_0 play very important roles in the director distribution in supertwist cells. The threshold voltage, its sharpness and the bistability can be changed by varying ϕ_t and θ_0 either independently or in combination.

In an ideal supertwist device, it would be desirable to have an extremely sharp threshold voltage and a small bistability [2]. Analysis of the computed data suggests that supertwist device with $\theta_0 = 5°$ and $\phi_t = 270°$ should provide the best performance characteristic with $\Delta\theta_m = 72°$ and a bistability $\Delta V = 0{\cdot}05$ V. However, such a low tilt device poses practical problems as 180° less twist mode configuration is also stabilized [4], resulting in a poor contrast. The formation of such a mode is restricted with increasing surface tilt angle. Larger surface tilt angles can support a larger twist angle without the formation of the scattering texture and 180° less twist mode. However, practically it is somewhat difficult to produce high tilt angle surfaces ($\theta_0 \approx 30°$) uniformly and economically over large areas. We have tried to optimize ϕ_t for intermediate surface tilt angle $\theta_0 = 15°$ so as to obtain an extremely large change in $\Delta\theta_m$ with a small bistability. Figure 4 shows the variation in the midplane

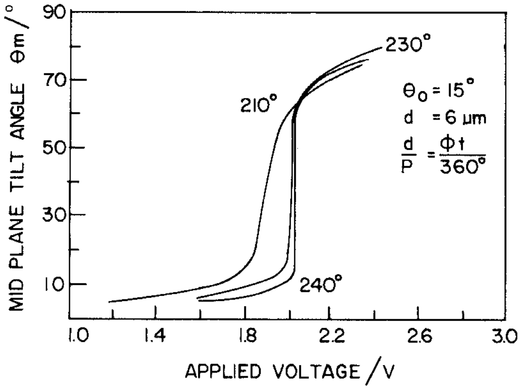

Figure 4. Variation of θ_m with the applied voltage in a supertwist cell with $\theta_0 = 15°$ for twist angles $\phi_t = 210°$, 230° and 240° with $d/p = \phi_t/360°$.

tilt angle as a function of the applied voltage in one such cell with $\theta_0 = 15°$ (which may be easier to realize practically) and $\phi_t = 210°$, 230° and 240°. It is immediately seen that a cell with $\theta_0 = 15°$ and $\phi_t = 240°$ would provide ideal conditions for the realization of a highly multiplexed display. As such, similar conditions could also be computed for other surface tilt angles.

3.5. *Influence of strained pitch*

In all of the previous computations, it was assumed that $p = (d/\phi_t) \times 360°$ (that is an unstrained pitch). However, in practice it may not be possible to meet this requirement rigorously. In the cell fabrication, ϕ_t is controlled by the surface alignment conditions and $p \neq (d/\phi_t) \times 360°$ (that is strained pitch). We have studied in detail the effect of varying the pitch p on the director distribution in cells with $\phi_t = 270°$, $\theta_0 = 30°$ and $d = 6\,\mu\text{m}$. Figure 5 shows the variation of the midplane tilt angle θ_m as a function of the applied voltage for the various values of p. It is clearly seen that in cells with $p > (d/\phi_t) \times 360°$ (the case of an understrained pitch) the bistability ΔV increases and the threshold voltage decreases with increasing pitch. Initially, the bistability increases somewhat linearly (see figure 6) with pitch but for $p > 9\,\mu\text{m}$, it increases very rapidly and as such the high energy on-state continues to exist even after the removal of the applied voltage. In this configuration the cell has an inherent memory which could be of great practical importance.

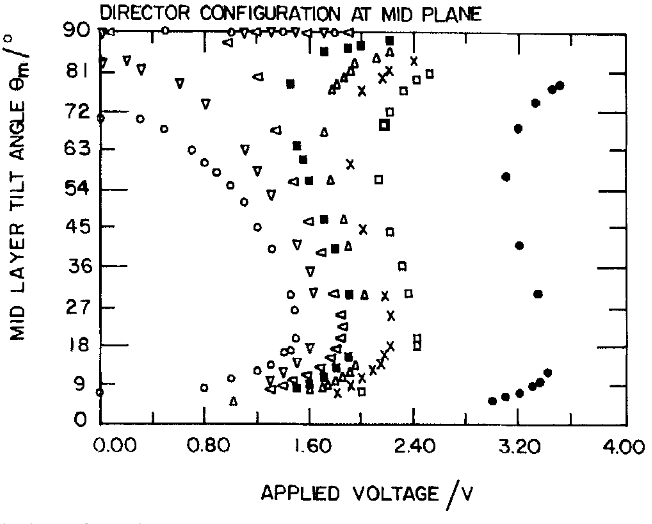

Figure 5. Variation of the θ_m with the applied voltage in supertwist cells with different pitch; $\phi_t = 270°$ and $\theta_0 = 30°$. Influence of a strained pitch (6 μm cell) for pitches of (●) 3, (□) 6, (x) 7, (△) 8, (■) 9, (◁) 10, (▽) 12 and (○) 15 μm.

For overstrained cells with $p < (d/\phi_t) \times 360°$, the bistability decreases and the threshold voltage increases with decreasing pitch. A new feature with respect to the threshold voltage is also observed in overstrained cells. It is found that the lower energy off-state solutions exist even beyond the threshold voltage corresponding to a uniform surface tilt orientation. It is difficult to explain this uncharacteristic behaviour beyond the usual threshold voltage V_{th}. The extension of the lower energy state beyond V_{th} may suggest the formation of another state which may be similar to

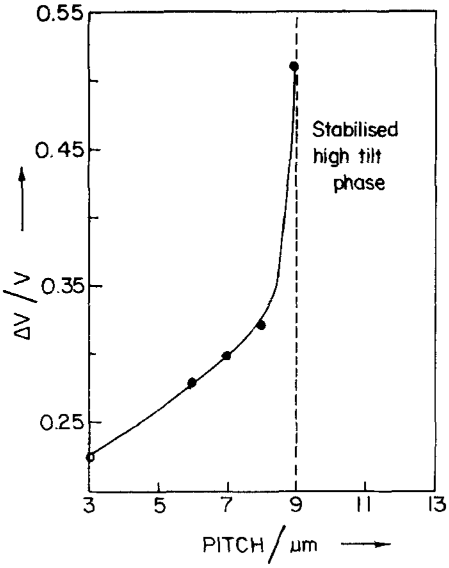

Figure 6. Variation of the bistability with the pitch p in supertwist cells with $\phi_t = 270°$ and $\theta_0 = 30°$.

the formation of stripe domains in real samples [7]. It is concluded from these computations that a proper choice of d/p together with ϕ_t and θ_0 would be of vital importance in controlling the director distribution and hence the optical performance characteristic in a supertwist cell.

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