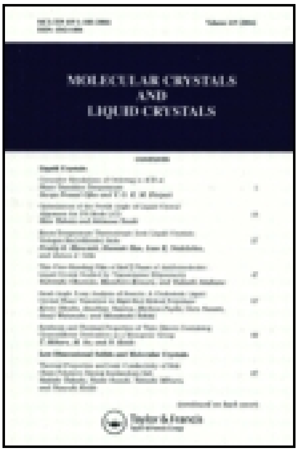

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Computational Calculations on the Chevron Structures in Ferroelectric Liquid Crystals

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In this paper we present numerical results for the chevron structure in a Surface Stabilized Ferroelectric Liquid Crystal (SSFLC) [1] sample. Using a phenomenological expression of the S_C bulk free energy and the numerical relaxation method, we calculate the spatial distribution of the director and the tilt of the layer in the chevron for twisted and uniform states for different applied voltages. In particular the results confirm the asymmetrical twist that has been observed in recent experiments.[2,3] The calculations take into account specific boundary conditions for both parameters with an applied electric field.

Keywords: Ferroelectric liquid crystals

1. INTRODUCTION

In most cases, the SSFLC sample induced a chevron structure that is derived from the layers shrinking due to the tilt of the optical axis: θ. Such a structure is modelled in the "nematic approximation" as a discontinuity of the layer tilt ($+\delta$, $-\delta$) for an uniform distribution of the director **n** (Figures 1–2): all molecules are parallel to the plate (*oxz* plane) and the nematic parameter does not show spatial distortion so that the energy is minimum.[4] But if one considers the azimuthal parameter φ describing the spatial distribution of the director, one finds a discontinuity. Thus, a soliton-like solution, where the disconitnuity has been replaced by a wall with a finite thickness, has been found to describe the structure.[5] The compression energy is then localized in a small region of the smectic layer. However, this analytical solution results from an approximation of the circular functions of the director. Experimentally, the variation of this parameter is large and its spatial distribution should be solved numerically.

2. CHEVRON STRUCTURE WITH PARTICULAR BOUNDARY CONDITIONS

The equilibrium equation[5] gives a soliton-like director distortion that is connected with the layer distortion independently of the boundary conditions; thus, the effective pretilt is estimated by consideration of the energy. In this model the anchoring torque is neglected relative to the bulk energy.

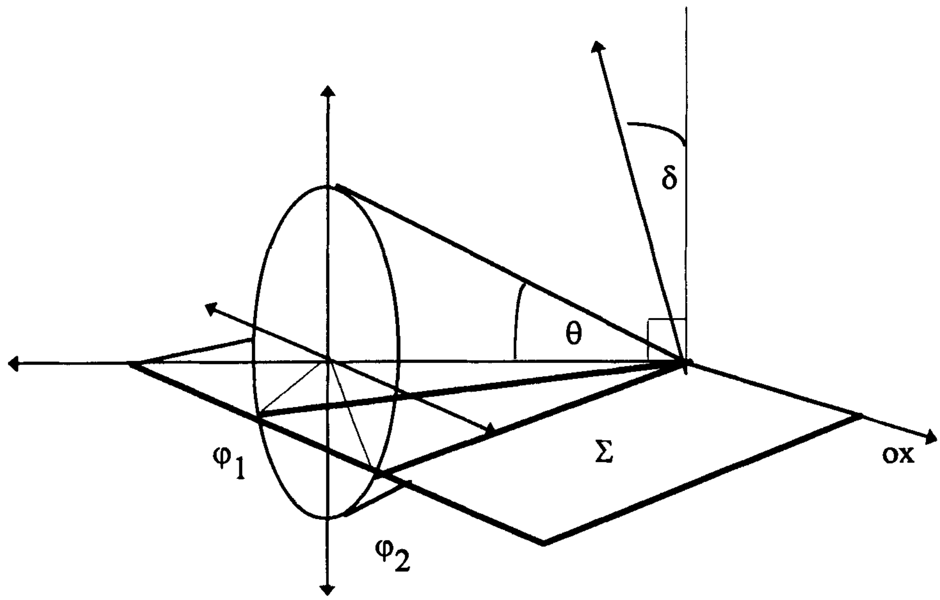

FIGURE 1 Boundary conditions of the director. Azimuthal angles at each plate: φ_1 or φ_2 are given by the intersection of the smectic cone and the plane of the electrode: Σ. δ is the tilt of the layer in the laboratory frame, θ is the tilt angle.

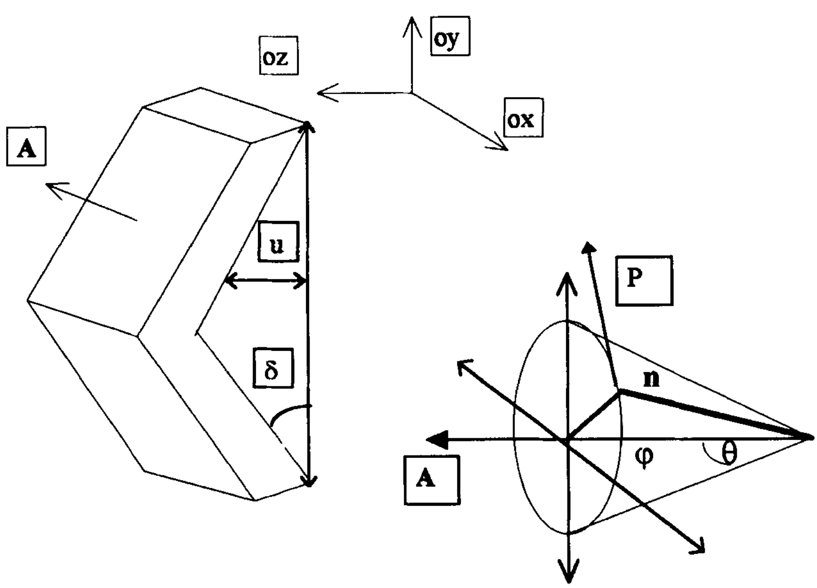

FIGURE 2 Geometry of the chevron structure. **A** is the layer normal defined in the laboratory frame, u is the layer displacement along the oz axis, φ is the azimuthal angle. **n** is the normalized director.

Experimentally it has been well proved that the tilt of the layer is independent of the surface treatment; however, one finds[6] that the thickness of the alignment film and the rubbing torque influence the apparent tilt angle. In the special case of a strong planar anchoring, geometrical considerations (Figures 1–2) give the value of the azimuthal angle: sing $\varphi = \delta/\theta$ on the plate.[6–8]

Generally, the tilts of the director and layers are of the same order of magnitude so that the apparent tilt of memorized states is very weak and leads to a lack of bistability. However, a large induced pretilt obtained by a particular alignment film treatment increases the apparent tilt and thus the bistability.

3. ANALYTICAL SOLUTION

For the layer parameters, we will use the derivatives of the layer displacement relative to ox and oy axes that give the layer normal. We also assume that in the chevron structure any layer compression in the oz direction can occur to preserve the density of layers in the SSFLC sample. The projection of the layer normal in the oxy plane is:

$$\vec{N}_\perp = \overrightarrow{\text{grad}}_\perp u = u = \begin{vmatrix} \dfrac{\partial u}{\partial x} \\ \dfrac{\partial u}{\partial y} \end{vmatrix}; \quad \text{the unit normal: } \vec{A}_\perp. \tag{3.1}$$

The quantity u is the layer displacement along the oz axis and $\delta = (\partial u/\partial y)$ (see Figure 2).

$$\text{The polarization vector is defined as } \vec{P} = P_0(\vec{A} \times \vec{n}). \tag{3.2}$$

In the case of the chevron structure, the variation of the parameters is along the oy axis thus, the phenomenological expression of the bulk free energy is given by:[9]

$$F = \frac{1}{2}\left(K_1\left(\frac{\partial\delta}{\partial y}\right)^2 + K_2\left(\frac{\partial\varphi}{\partial y}\right)^2 + 2C\left(\frac{\partial \sin\varphi}{\partial y}\right)\left(\frac{\partial\delta}{\partial y}\right)\right) + B/4\cdot(\delta^2 - \Theta^2)^2. \tag{3.3}$$

The energy involves two different categories: the elastic energy for both orientation parameters (first three terms) and the layer compression energy where Θ is a parameter of the same order of magnitude as the tilt angle.

Minimizing the energy one obtains the equilibrium equations:

$$\begin{aligned} K_1\delta_{yy} + C(\sin\varphi)_{yy} &= B\delta(\delta^2 - \Theta^2) \\ K_2\varphi_{yy} + C\delta_{yy}\cos\varphi &= 0. \end{aligned} \tag{3.4}$$

For small variations of the director, circular functions can be approximated to the first order. With the transformations

$$\lambda = \left(\frac{K_1}{B}\right)^{1/2} \quad \rho = 1 - \frac{C^2}{K_1K_2} \tag{3.5}$$

one finds the typical soliton-like solution for δ and φ:[5]

$$\delta = \Theta \tanh\left(\frac{\Theta y}{2\sqrt{\rho\lambda}}\right); \quad \varphi = \frac{C}{K_2}\Theta \tanh\left(\frac{\Theta y}{2\sqrt{\rho\lambda}}\right) + \alpha y. \tag{3.6}$$

The kink solution for the director does not take into account the boundary conditions at each plate: $\varphi = (\Theta/\theta)$. Experimentally, the tilt of the director is of the same order of magnitude as the tilt of the layer thus with such boundary conditions, we could not approximate the circular functions of the differential system. In the case of a twisted state where the azimuthal angle has a large variation (180°), the approximation is even less applicable and one must use the system 3.4.

4. NUMERICAL COMPUTATIONS

In this section we shall present numerical solutions of the system 3.4 for the uniform and twisted distribution of the director. With such a method it is possible to include the coupling between an external electric field E_y and the spontaneous polarization P_0. The coupling energy expression is as follows:

$$\Pi = -P_0 E_y \cos\delta \cos\varphi. \tag{4.1}$$

With the external electric field, the equilibrium equations are rewritten as:

$$\begin{cases} \delta_{YY} + \Omega(\sin\varphi)_{YY} = \delta(\delta^2 - \Theta^2) + \varepsilon \sin\delta\cos\varphi \\ \delta_{YY}\cos\varphi + \Gamma\varphi_{YY} = \dfrac{\varepsilon}{\Omega}\sin\varphi\cos\delta \end{cases} \tag{4.2}$$

with the normalized quantities:

$$\Omega = \frac{C}{K_1}, \quad \Gamma = \frac{K_2}{C}, \quad \varepsilon = \frac{P_0 E}{B}, \quad y = \sqrt{\frac{K_1}{B}}Y.$$

With the transformation: $(\sin\varphi)_{YY} = -\sin\varphi(\varphi_{YY})^2 + \cos\varphi\,\varphi_{YY}$; the differential system leads to equations:

$$\begin{aligned} \delta_{YY} &= \frac{1}{\Delta}\left(-\Gamma\left(\delta(\delta^2 - \Theta^2) + \Omega\sin\varphi(\varphi_Y)^2 + \varepsilon\sin\delta\cos\varphi\right) + \varepsilon\sin\varphi\cos\delta\right) = f(y) \\ \varphi_{YY} &= \frac{1}{\Delta}\left(\cos\varphi(\delta(\delta^2 - \Theta^2) + \Omega\sin\varphi(\varphi_Y)^2 + \varepsilon\sin\delta\cos\varphi) - \frac{\varepsilon}{\Omega}\sin\varphi\cos\delta\right) = g(y) \end{aligned} \tag{4.3}$$

with $\Delta = \Omega\cos^2\varphi - \Gamma$.

For practical computation, taking difference forms, the differential terms could be written as:

$$\delta_{YY}=\frac{\delta(I+1)-2\delta(I)+\delta(I-1)}{h^2} \quad \text{and} \quad \varphi_{YY}=\frac{\varphi(I+1)-2\varphi(I)+\varphi(I-1)}{h^2} \tag{4.4}$$

where "h" is a finite element of length.
One calculates the I^{th} terms of the second order partial derivative versus $f(I)$, $g(I)$ and the $I+1^{\text{th}}$, $I-1^{\text{th}}$ terms of second order partial derivatives:

$$\begin{aligned}\delta(I)&=\frac{1}{2}(-f(I)\cdot h^2+(\delta(I+1)+\delta(I-1)))\\ \varphi(I)&=\frac{1}{2}(-g(I)\cdot h^2+(\varphi(I+1)+\varphi(I-1))).\end{aligned} \tag{4.5}$$

One solves the system by the iterative method. First, one makes the choice of initial approximated functions that are put in the left-hand part of (4.3). The newly calculated values of both parameters (left-hand side) are then inserted to the right-hand side. The convergence of iterations leads to the exact answer.[10]

5. RESULTS

5.1 Uniform States

Assuming that at each plate the azimutal parameter φ remains constant and one imposes a drawn derivatives for the tilt of the layer δ at the same place, one obtains solutions very similar to those with the approximations of the first order circular functions (see Figure 3). The distribution of the azimuthal angle is analogous to the superposition of a uniform twist and a soliton-like distribution: the coupling between layer and director tilt always induces a distortion at the chevron interface.

5.2 Twisted States

In the particular case where the anchoring to the plate is polar, a twisted structure appears in the bulk. Usually, such a structure is represented as a uniform twisted distribution of the director. However, optical observations show an asymmetrical distribution of the azimuthal parameter in the chevron. Moreover, calculations of perturbations validate this behaviour near the chevron interface.[9] Numerical computations also confirm these results and show an asymmetrical spatial distribution of φ which depends highly on the normalized constant: Γ (Figure 4). For high values of this constant, the distribution tends to the symmetrical structure (uniform twist) because the coupling between the director and the tilt of the layer decreases. This distribution of the director is analogous to that in the bookshelf structure. Moreover, the largest variation of the director could be localized in each part of the chevron, (the

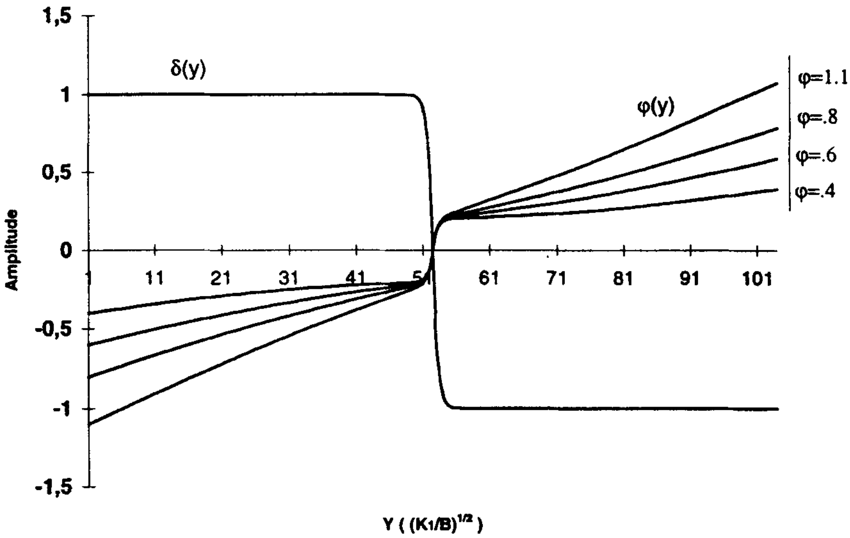

FIGURE 3 Uniform states, with different boundary conditions for the azimuthal parameter. $\phi = .4, .6, .8, 1.1$; $\Omega = .1$, $\Gamma = 5$; Amplitude is expressed in rad for φ, δ is normalized.

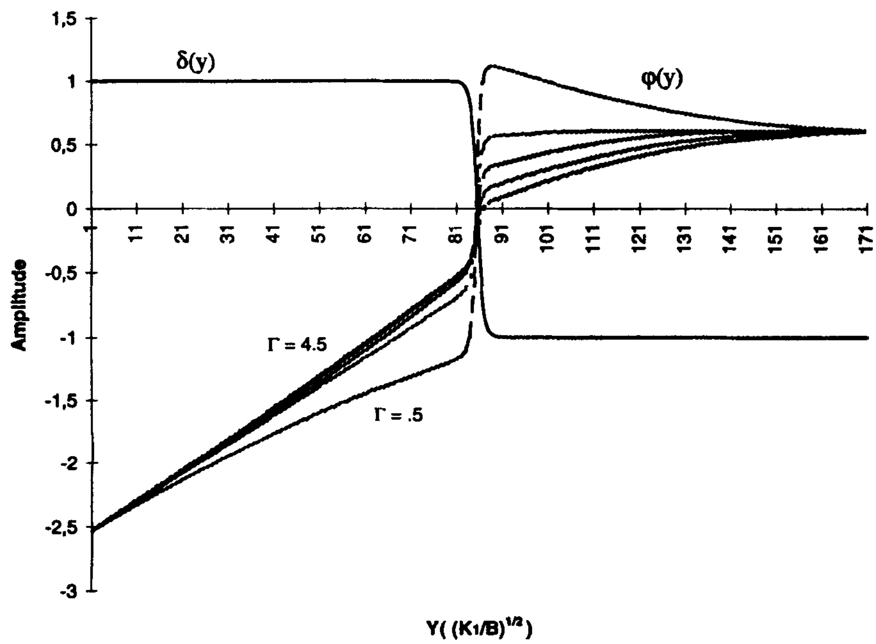

FIGURE 4 Twisted states for different values of the normalized constant $\Gamma = 4.5, 2.5, 1.5, .5$, $\Omega = .1$. For the large value, the spatial distribution of the director tends to be uniform. Amplitude is expressed in rad for φ, δ is normalized.

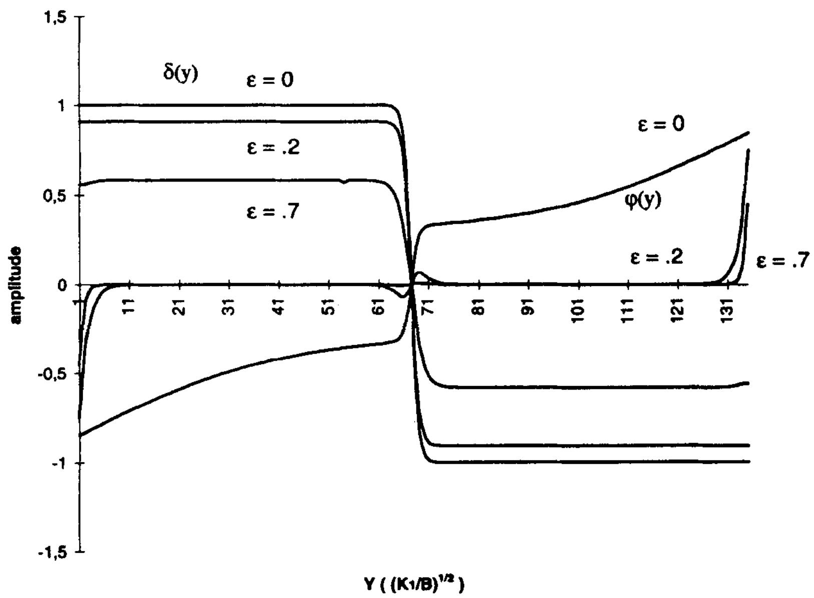

FIGURE 5 Uniform states with an external electric field: $\varepsilon = 0; .2; .7$. Amplitude is expressed in rad for φ, δ is normalized.

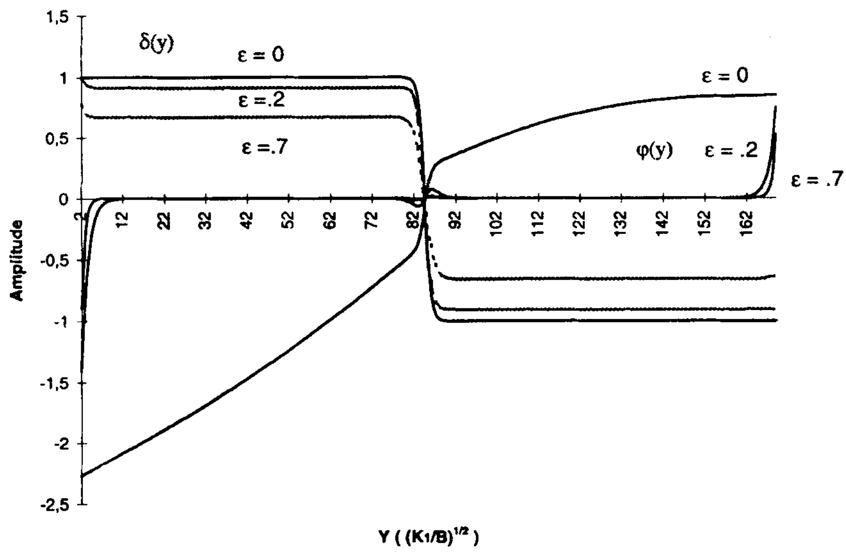

FIGURE 6 Twisted states with an external electric field: $\varepsilon = 0; .2; .7$. Amplitude is expressed in rad for φ, δ is normalized.

azimuthal parameter could then be locked at 0 or π at the chevron interface) thus, two configurations are possible.

5.3 Uniform and Twisted States with an Electric Field

The coupling energy with the external electric field could change the spatial distribution of both parameters δ and φ (see Figures 5 and 6). The director orientation rapidly tends toward zero in the bulk and the tilt of the layer progressively decreases. However, for the asymmetrical twist distribution, one observes a small distortion of δ for the high value of the electric field near the boundaries. This kind of distortion appears in that part of the chevron where the distance covered for φ is the longest.

For an upper electric field, the tilt of the layer decreases quickly and then the azimuthal angle vanishes at the boundaries. The drawn derivative of the tilt of the layer is still preserved. For uniform states the distortion of the φ parameter is lower and does not induce layer tilt distortion.

6. CONCLUSION

The computational method of relaxation gives satisfying results on the director and the tilt of the layer distribution with or without application of electric field. The asymmetrical twist structure is confirmed and the azimuthal parameter remains locked to the $\varphi = 0$ or π position in the middle of the chevron. However, the boundary conditions were chosen for geometrical considerations and with the assumption that the tilt of the layer is free near the plate. Such conditions remain to be justified (or quashed) with a deeper knowledge and understanding of the anchoring effect.

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