Calculation of chevron profiles in ferroelectric liquid crystal cells

Arnout De Meyere[ab]; Herman Pauwels[a]; Erwin De Ley[ac]

[a] Laboratory of Electronics, University of Gent, Gent, Belgium [b] Belgian National Fund for Scientific Research (NFWO), [c] Institute for Scientific Research in Industry and Agriculture (IWONL),

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Calculation of chevron profiles
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by ARNOUT DE MEYERE*†, HERMAN PAUWELS and ERWIN DE LEY‡

Laboratory of Electronics, University of Gent,
Sint-Pietersnieuwstraat 41, B-9000 Gent, Belgium

The energetic aspects of layer deformation in ferroelectric liquid crystal cells are discussed and the actual chevron shape is calculated in some situations. We emphasize two, in our view, essential energy contributions. One term considers the layer curvature. The other one refers to the variations in the distance between layers and the consequent changes of the smectic cone angle. In some simple cases we can determine optimal shapes of the chevron layer structure by analytical solutions, based on these two energy terms. In more complicated situations other contributions have to be considered and the chevron profiles are simulated numerically. The influence of the applied voltage and the choice of parameter values are studied.

1. Introduction

Since the invention of surface-stabilized ferroelectric liquid crystals [1], the chiral smectic C layer structure in these displays has been a hot topic of research and discussion. After high resolution X-ray and optical response measurements, the first model with bookshelf geometry was modified to describe inclined and bent layers [2–4]. Important adjustments of the theory came with the introduction of the chevron structure [5–7]. Geometrical consequences (such as zig-zag defects) and the influence of alignment layers and temperature were studied in further detail (see, for example [8, 9]). Research has continued and more exotic variations of the chevron layers have been published recently [10, 11]. Meanwhile, theoretical energy specialists such as Dahl [12, 13] and Nakagawa [14, 15] have refined the energy expressions, useful for numerical modelling.

The aim of this paper is mainly to present analytical and numerical ways for the study of the optimal shape of one-dimensional chevrons. Should the chevron interface be considered as discontinuous or smooth? Also the influence of an applied electric field on the layer profile is a topic of discussion. How and to what extent are the layers bent by the torque that exists on each molecule through its polarization vector? Extensive layer bending has been suggested in the literature (see, for example [16]). However, few attempts have been made to develop energetical verification of the layer bending model. MacGregor [17] has made an important numerical analysis, based on the energy expressions of Dahl. But he neglected one energy term which seems very important to us: the energy cost of the layer bending and its implications on the layer thickness and the smectic cone angle. We will also discuss more recent work by Willis *et al.* [18] on the layer response to low electric fields. In any case, it may be clear that chevron shapes are crucial for grey-scale techniques [19]. Variations of the chevron

* Author for correspondence.
† Supported by the Belgian National Fund for Scientific Research (NFWO).
‡ Supported by the Institute for Scientific Research in Industry and Agriculture (IWONL).

layer structure are in fact deviations of the positional ordering in layers. The classical Oseen–Frank energy expressions only refer to orientational ordering of the molecules. In §2 we consider two, in our view, essential new energy terms: one expresses the curvature of the layers, and the other takes account of variations in distance between layers and thus changes in the cone angle. We also make an attempt to derive the proposed energy terms from the general expressions, that are developed by Dahl [12, 13, 20]. In §3, we limit ourselves to a simple case where exact analytical solutions can be found. Variations of the layer structure depend only on the coordinate which is perpendicular to the glass surfaces. We search for the two stable states where the molecules are parallel to the glass surfaces. In §4, we consider the same one-dimensional situation as in §3, but now the influence of a voltage over the display is taken into account. Analytical solutions are no longer possible. The computer program is rather complicated, and its principles are explained. Some results are discussed. In §5, we try to generalize some of our results to variations in two dimensions. When an electric field tends to orient the polarization as perpendicular as possible to the glass surface, bending occurs in the direction perpendicular to the rubbing direction. Such structures were proposed in the literature [10, 11]. We show that these structures are in agreement with the energy terms under consideration. They are the only structures that minimize cone angle variations. Exact analytical solutions are no longer possible, and adaptations of the computer program to two-dimensional cases are not performed yet.

2. Energy expressions

In figure 1, one can see the coordinate systems that we used. The *xyz* system is the reference frame with the *x* axis perpendicular to the glass plates, and the *z* axis parallel to the rubbing direction. The *cpk* system is used for calculating elastic energies according to the expressions of Dahl [13, 20]. The k axis is the smectic cone axis. Note that we do not allow arbitrary orientation of the cone: k always lies in the *xz* plane. Further rotation of *cpk* delivers the classical 123 or *qpn* axes connected with the liquid
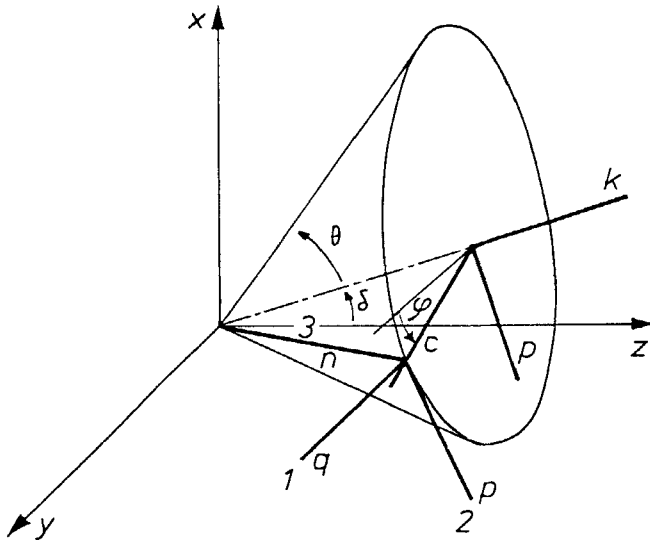

Figure 1.   The coordinate systems used to describe the FLC structure. Both the *cpk* and the *qpn* systems occur in the energy calculations.

crystal molecule. The coordinates of **n** are used in the normal Oseen–Frank expressions. Three angles (φ, δ and θ) govern the structure. Without giving any details, we can calculate the following energy contributions, in case the angles only vary along the x direction (one dimensional approach).

2.1. *Volume energy*

Three contributions to the volume energy have to be considered: the elastic part, the cone angle deviation energy and the electric term.

2.1.1. *The elastic energy*

(*a*) A first option is to use a modified form of the Oseen–Frank elastic energy. The classical Oseen–Frank expression only considers the orientational ordering of the molecules. In order to take the smectic structure into account we propose to introduce an additional term. Indeed, the layer bending causes the molecules to be displaced from their favourite position. In our one-dimensional approach, the layer bending can be described by the first derivative of the angle δ. We suggest the energy term $A\delta_x^2$. The index x indicates derivation towards the x-coordinate.

If we consider equal elastic constants ($K_1 = K_2 = K_3 = K$) and $q_{\parallel} = q_{\perp} = 0$, we obtain

$$
\begin{aligned}
f_{\text{elas}} &= A\delta_x^2 + \tfrac{1}{2}K((\nabla \cdot \mathbf{n})^2 + (\nabla \times \mathbf{n})^2) \\
&= A\delta_x^2 + \tfrac{1}{2}K(\sin^2 \theta)\varphi_x^2 + (1 - \sin^2 \theta \cos^2 \varphi)\delta_x^2 + \theta_x^2 \\
&\quad - 2\sin\theta\cos\theta\cos\varphi\varphi_x\delta_x - 2\sin\varphi\delta_x\theta_x.
\end{aligned} \tag{1}
$$

(*b*) A second possibility is to start from the expressions according to Dahl–Lagerwall [13, 20],

$$
f^{\bullet}_{\text{elas}} = f_s + f_c + f_{cs} + f_* + f_g. \tag{2}
$$

Here the smectic layer bending has already been taken into account. In our coordinate system, we calculated the following expressions for the basic terms in Dahl's energy equations (see [13]).

$$
\begin{aligned}
t_{11} &= -\sin\varphi\cos\varphi\cos\delta\delta_x, \\
t_{21} &= -\cos^2\varphi\cos\delta\delta_x \\
t_{31} &= \cos\varphi\sin\delta\delta_x, \\
t_{12} &= -\sin^2\varphi\cos\delta\delta_x, \\
t_{22} &= \sin\varphi\cos\varphi\cos\delta\delta_x, \\
t_{32} &= -\sin\varphi\sin\delta\delta_x, \\
t_{13} &= -\sin\varphi\cos\delta\varphi_x, \\
t_{23} &= -\cos\varphi\cos\delta\varphi_x, \\
t_{33} &= \sin\delta\varphi_x.
\end{aligned}
$$

Now we combine these terms according to [13]. We neglect the so-called gauge terms ($f_g = 0$), and after strong reduction of parameters

$$(A_{11} = 4\mathscr{A},\; A_{12} = A_{21} = A_{31} = A_{32} = 2\mathscr{A},\; A_4 = A_6,\; A_5 = 0,\; \bar{B} = 0$$

$$B_1 = B_2 = B_3 = \mathscr{B},\; B_{13} = 0,\; C_1 = C_2 = C_3 = \mathscr{C},\; C_4 = 0,\; D_1 = D_2 = D_3 = \mathscr{D})$$

we find

$$
f^{\bullet}_{\text{elas}} = \mathscr{A}\delta_x^2 + \mathscr{B}\varphi_x^2 + \mathscr{C}\cos\varphi\varphi_x\delta_x + \mathscr{D}(\sin\delta - \sin\varphi\cos\delta)(\varphi_x + \cos\varphi\delta_x) \tag{3}
$$

(comparable simplifications were made by MacGregor [17]).

Note the difference between A in equation (1) and $\mathscr{A}$ in equation (3). In the last equation, $\mathscr{A}$ is the coefficient of the unique δ_x^2 term which takes care of both the layer bending and the director distortion. In equation (1), A only refers to the layer bending energy. The term $\bar{B}\gamma^2$ in the Dahl–Lagerwall expressions [20] which deals with the compression (or distension) of the layers has not been included. It will be replaced by a similar term (see equation (5)).

The first term in equation (3) describes the deformation of the smectic layers, the second one handles the energy cost of the molecule turning on the smectic cone and the third contribution takes the coupling of these two into account. The last term takes care of the chiral energy. For this paper, we have studied the energy form (3) in an even more simplified form. We neglect the chiral term ($\mathscr{D} = 0$) and we assume φ to be close to zero. Since important conclusions will be drawn in the case of an applied field, this is not an unpermitted assumption. As soon as an electric field is applied, the molecules turn to their favourite position on the smectic cone, as can be seen on the simulations in figure 6. We are aware of the inaccuracy and plan to investigate the full terms later. The calculations are simplified by taking for the elastic energy:

$$f_{\text{elas}}^{\bullet} = \mathscr{A}\delta_x^2 + \mathscr{B}\varphi_x^2 + \mathscr{C}\varphi_x\delta_x \tag{4}$$

2.1.2. *The cone angle deviation energy*

For the cone angle deviation energy we considered the first term of the Landau expansion

$$f_{\text{cone}} = T\sin^2(\theta - \theta_{\text{e}}) \tag{5}$$

where θ_{e} indicates the equilibrium value for θ.

2.1.3. *The electric energy*

For the electric energy the calculation method simplifies when the dielectric displacement D is taken as parameter. The corresponding voltage drop across the liquid crystal layer is then obtained from the equilibrium angle distribution. This means that we consider the Helmholtz free energy (compare Pauwels *et al.* [21] or Wöhler *et al.* [22]):

$$f_{\text{elec}} = \tfrac{1}{2}ED_{\text{e}}$$
$$= \tfrac{1}{2}\epsilon_0\epsilon_{xx}E_x^2 \tag{6}$$

As a summary for the volume energy, we have the choice between two expressions, depending on the choice of the elastic energy.

(*a*) With Oseen–Frank

$$f_{\text{volume}} = A\delta_x^2 + \tfrac{1}{2}K((\nabla\cdot\mathbf{n})^2 + (\nabla\times\mathbf{n})^2) + T\sin^2(\theta - \theta_{\text{e}}) + \tfrac{1}{2}\epsilon_0\epsilon_{xx}E_x^2. \tag{7}$$

(*b*) With Dahl–Lagerwall

$$f_{\text{volume}}^{\bullet} = \mathscr{A}\delta_x^2 + \mathscr{B}\varphi_x^2 + \mathscr{C}\varphi_x\delta_x + T\sin^2(\theta - \theta_{\text{e}}) + \tfrac{1}{2}\epsilon_0\epsilon_{xx}E_x^2. \tag{8}$$

2.2. *Surface energy*

With $\mathbf{s}$ the outward normal to the glass-plates, $\mathbf{n}$ the director and $\mathbf{p}$ the unit polarization vector, we can write

$$f_{\text{surf}} = \gamma_1(\mathbf{n}\cdot\mathbf{s})^2 - \gamma_2(\mathbf{p}\cdot\mathbf{s}). \tag{9}$$

Equations (8) and (9) are the starting point for a minimization program, described in §4. At this point, however, one very important refinement is still necessary; this was already mentioned in the first chevron papers (see, for example, [6] and [7]), but is sometimes neglected in literature ([17]).

Variations of the smectic layer structure, through variations of the angle δ often lead to changes of the layer thickness. This means that the cone angle has to deviate from its equilibrium value. The situation is clarified in figure 2.

The following relations are easily verified:

$$\left. \begin{aligned} d_\perp &= l\cos\theta \\ &= d_z\cos\delta, \\ \cos\theta &= v\cos\delta, \end{aligned} \right\} \tag{10}$$

with

$$v = \frac{d_z}{l}, \tag{11}$$

where l is the molecular length and d_z the distance between the layers along the z-axis, the rubbing direction. This parameter d_z is in fact determined by the way the transition from smectic A to smectic C occurred. Notice that the number of molecules between two layers is in fact determined by this parameter, since it defines the volume between the layers.

Equation (10) indicates a coupling between δ and θ. Especially in the one dimensional approach which we are dealing with, d_z has to be constant. Hence, in this case each variation of δ causes variations of θ, which are very hard to establish. Therefore, in equation (8) there are only two independent variables, φ and δ. The connection between δ and θ would lead to even more mathematical complications if one proceeds from the Oseen–Frank equations (1).

At this point, we want to refer to an important recent article by Willis *et al.* ([18]). The authors conclude after X-ray measurements that 'The chevron rules are satisfied globally, but violated locally'. This would mean that rule (10) is not satisfied locally. We agree that this can be the major objection to our research. However, since there is no
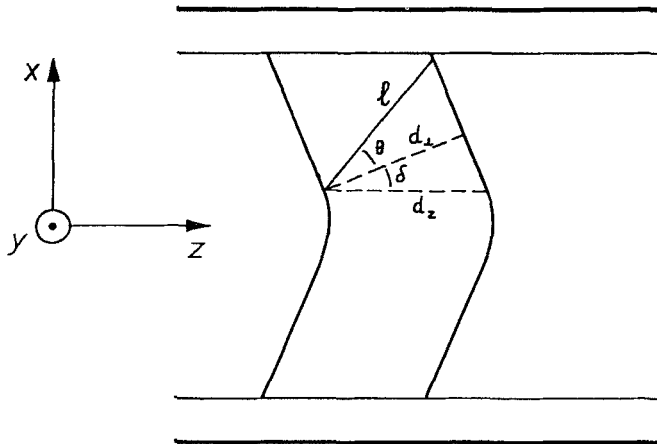

Figure 2.   In the one dimensional approach, there exists a fixed relation between the cone angle θ and the layer tilt δ.

rigorous explanation at this point (Willis *et al.* suggest the presence of layering defects, maybe edge dislocations), we think that it is useful to investigate the predictions of the defect-free theory. In any case, the x dependence of the angle δ ($=$ layer bending) is more accurately dealt with here than in [18] where an average value for δ is used.

3. One dimensional analytical solution

From figure 1 we can deduce the coordinates of the director **n** with respect to the xyz-frame

$$\mathbf{n} = \mathbf{l}_x[-\sin\theta\sin\varphi\cos\delta + \cos\theta\sin\delta]$$

$$+ \mathbf{l}_y[\sin\theta\cos\varphi]$$

$$+ \mathbf{l}_z[\sin\theta\sin\varphi\sin\delta + \cos\theta\cos\delta]. \tag{12}$$

If the director is parallel to the glass surface, its φ-angle is given by

$$\sin\varphi = \frac{\tan\delta}{\tan\theta} \tag{13}$$

and its angle ψ with the z-axis

$$\cos\psi = \frac{\cos\theta}{\cos\delta}. \tag{14}$$

Using our important equation (10) we see that $\cos\psi = v$, independent of x. So, in the two stable states, all the molecules are parallel to each other (and to the glass surface). The Oseen–Frank energy (second term in equation (1)) for these states is thus zero and minimal. Unfortunately the polarization is x-dependent for these states

$$P_x = -P\cos\varphi\cos\delta. \tag{15}$$

In absolute value, this expression will be minimal at the glass surface and maximal ($=P$) in the middle. Even when there is no voltage over the liquid crystal, there will be an x-dependent electric field. Therefore the electrostatic energy, (*) for constant D (Helmholtz free energy): $\frac{1}{2}\epsilon_0\epsilon_{xx}E^2$, (**) or for constant V (Gibbs free energy): $-\frac{1}{2}ED_e - EP$ (see [21]), is not zero. In this section, we shall neglect this effect. The optimal form of the layers, under short-circuit, is then determined by minimization of the positional energy. So, we can deduce from (7) the simplest form of the energy to be minimized, with $\frac{1}{2}K((\nabla\cdot\mathbf{n})^2 + (\nabla\times\mathbf{n})^2) = 0$

$$\gamma = \int\left[A\left(\frac{d\delta}{dx}\right)^2 + T\sin^2(\theta - \theta_e)\right]dx. \tag{16}$$

The first term takes account of the deviation of the layers from a planar configuration, and the second term considers the deviations of the cone angle from its equilibrium value. Since equation (10) describes how θ varies with x through δ, the second term basically can be expressed as a function of δ. So we end up with:

$$\gamma = \int\left[A\left(\frac{d\delta}{dx}\right)^2 + g(\delta)\right]dx. \tag{17}$$

In figure 3 the dependence of δ and g on x are schematically represented.

As shown in the appendix, γ is minimal for

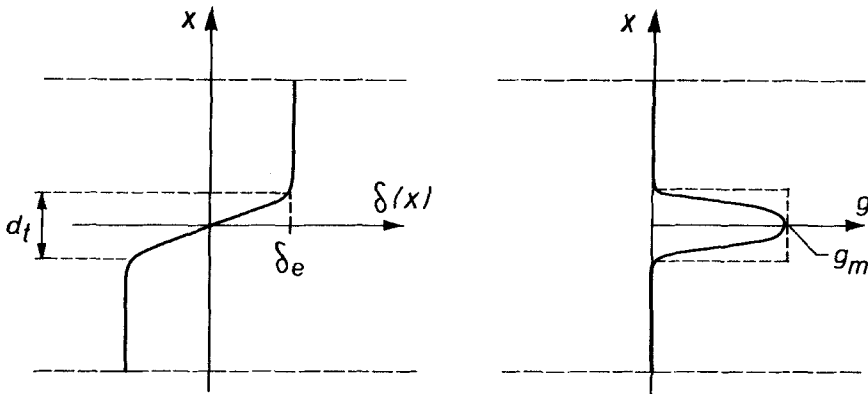$$A\left(\frac{d\delta}{dx}\right)^2 = g(\delta) \tag{18}$$

Figure 3. Dependence of the layer tilt δ and the cone angle variation energy g on x.

and this minimal value is given by

$$\gamma = 2\sqrt{A} \int_{-\delta_e}^{\delta_e} \sqrt{[g(\delta)]}\, d\delta \tag{19}$$

A simple approximation shows more clearly what happens. In the middle of the liquid crystal, the cone angle has its minimum value, $\cos \theta_m = v$. There the cone angle energy has its maximum value $g_m = T\sin^2(\theta_m - \theta_e)$. If we now assume that g jumps to its maximum value, as soon as δ deviates from its equilibrium value, then equation (18) shows that $d\delta/dx$ is constant in this region.

If this region has a thickness d_t then

$$\frac{d\delta}{dx} = 2\frac{\delta_e}{d_t} \tag{20}$$

and

$$\gamma = A\frac{4\delta_e^2}{d_t^2}d_t + g_m d_t, \tag{21}$$

which is minimal for

$$d_t = 2\sqrt{\left(\frac{A}{g_m}\right)}\delta_e \tag{22}$$

and

$$\gamma_{min} = 4\sqrt{(Ag_m)}\delta_e. \tag{23}$$

Equation (22) describes the thickness of the tip of the chevron layer. We no not know the relative values of the constants A and T. However, most researchers assume on experimental grounds that the tip of the chevron layer is very small, so we must accept that T is much more important than A. The transition in δ from δ_e to $-\delta_e$ occurs almost discontinuously, such that the energy stored in the 'deviation from a plane' is still as important as that stored in the 'cone-angle deviation'. Because the chevron tip is so thin, we also dared to neglect the electrostatic free energy at zero voltage. The polarization charge and field distribution are schematically represented in figure 4. The effect of the double layer disappears when d_t goes to zero.
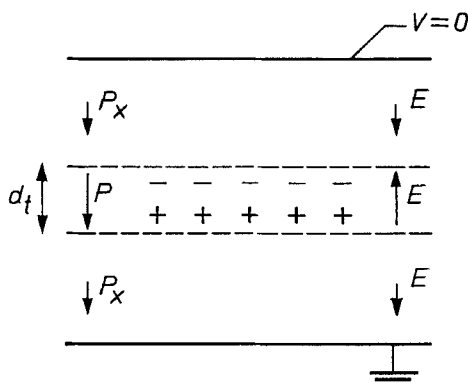
Figure 4. Even under short circuit conditions, the orientation of the polarization vector changes through the layer. This corresponds with the presence of polarization charge.

4. Numerical approach

A common method to handle structural problems like this goes as follows: one derives the so-called Euler–Lagrange equations from the energy functional (with expressions (8) and (9) as integrand) and looks for the time independent solutions. MacGregor (see [17]) uses this method in a successful way, but without considering the δ–θ coupling.

Another method, rather straightforward in principle, has been suggested already in Karlruhe (see, for example, Wöhler *et al.* [22]). One divides the liquid crystal layer into slabs and uses a linear approximation for the two angles (φ and δ in our case) within each slab. In this way, the energy integral can be reduced to a function of the node values, which has to be minimized. A modified multi-dimensional Newton–Raphson method is used to calculate the angle distributions that minimize the energy. Programs have been made with this numerical method, but as far as we know only for the easier case of nematic liquid crystals. Also, at our laboratory, such a program is being used (see [23]). We adapted the program for the more complicated energy expressions. In this article we want to share our first results.

In figure 5 one can see the influence of the applied voltage on the chevron tip width. We had to choose numerical values for the different parameters in expressions (8) and (9): $\mathscr{A} = 10\,\text{pN}$, $\mathscr{B} = 1\,\text{pN}$, $\mathscr{C} = 1\,\text{pN}$, $T = 100\,000\,\text{Pa}$, $P = -300\,\mu\text{C m}^{-2}$, $\gamma_1 = 100\,\mu\text{N m}^{-1}$ and $\gamma_2 = 50\,\mu\text{M m}^{-1}$ (for order of magnitude see also MacGregor [17]). As a measure of tip width, we calculated the region in the liquid crystal where δ deviates more than 10 per cent from its equilibrium value at the border. Indeed, bending of the layers occurs after application of the voltage drop.

The extent of the bending is largely dependent on the magnitude of our constants. If we decrease the T constant (for the cone angle deviation or soft mode) by one order of magnitude to $10\,000\,\text{Pa}$, the influence of the electric field on the layer profile is much larger, as illustrated in figure 6. In other words, layer bending is large in the case of small compression energy. This is only an illustration of our numerical results. X-ray data (see [18]) seem to illustrate that T should be taken as fairly large. In that case, the layers bend just very slightly, as indicated in figure 5. Note that both δ and φ are plotted in figure 6: the upper three curves show the variation of δ in the upper half of the liquid crystal layer, for three different values of the voltage. The lower three curves show φ to be equal to zero almost everywhere (a small voltage sucks the molecules to their favourite position on the cone, see figure 1).
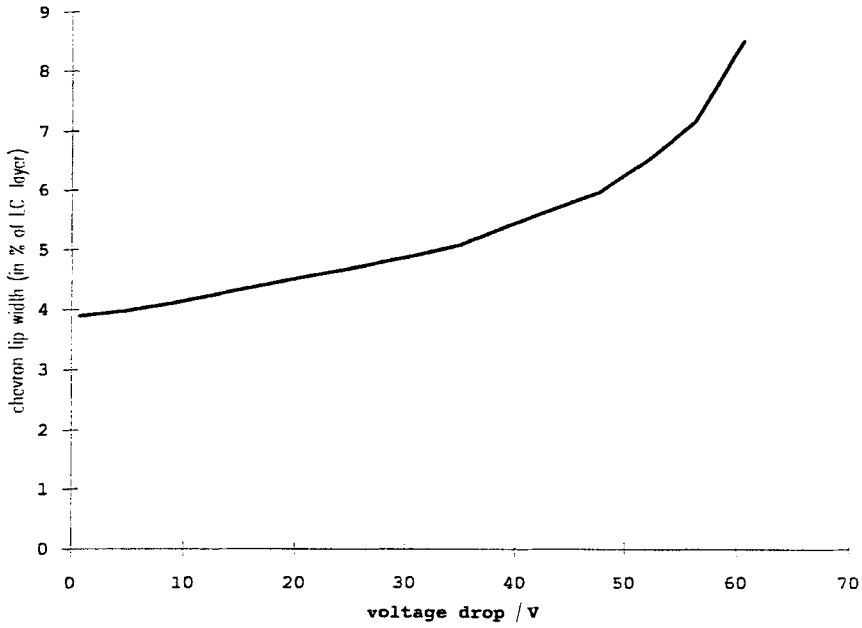
Figure 5.   The chevron tip width increases with the applied voltage drop.
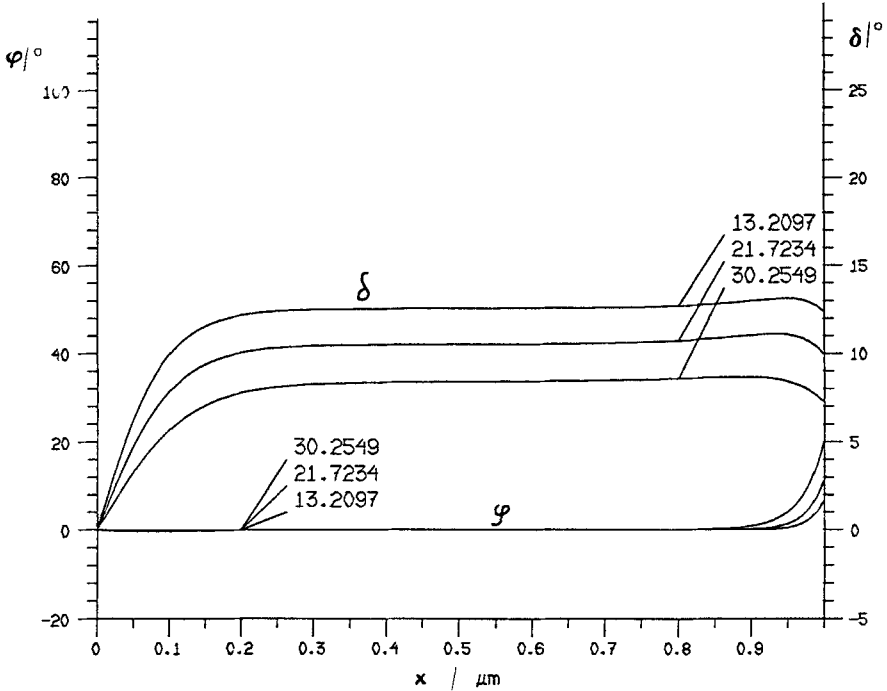

Figure 6.   For relatively small values of T, the layers bend easily, as can be seen from the curves. The indicated curve parameter is the corresponding voltage drop. The angle distributions are shown in the case $T = 10\,000$ Pa.

Finer analysis of experimental data might lead to the realistic values for our parameters. But it is our feeling that T could possibly be so large that bending is far less obvious than has been assumed up till now in literature.

5. Two dimensional structures

In the one dimensional case, it is not possible to influence drastically the form of the chevron layer through the electric field. Although in the tip of the chevron layer the polarization is more aligned with the electric field, the cone angle is decreased. The energetical disadvantage of the last effect causes the tip of the chevron to remain very small. In the recent literature ([10, 11]), structures were proposed in which the layers have an inclination δ_e with respect to the y-axis instead of the x-axis. An example is demonstrated in figure 7. The distance between layers along the z-axis remains unchanged, so that the number of molecules between layers is unchanged. Now the polarization can become perpendicular to the glass surface, without changing the cone angle, so that these states are favoured by the electric field. Some of these structures only require displacements of molecules in the bulk of the liquid crystal, which are considered to be reversible, but other structures include displacements of molecules at the glass surface, which are irreversible, and therefore stable.

Suppose the shape of the layers is described by a function $z(x, y)$ with partial derivatives.

$$\left.\begin{array}{l} u = \dfrac{\partial z}{\partial x}, \\[3mm] v = \dfrac{\partial z}{\partial y} \end{array}\right\} \qquad (24)$$
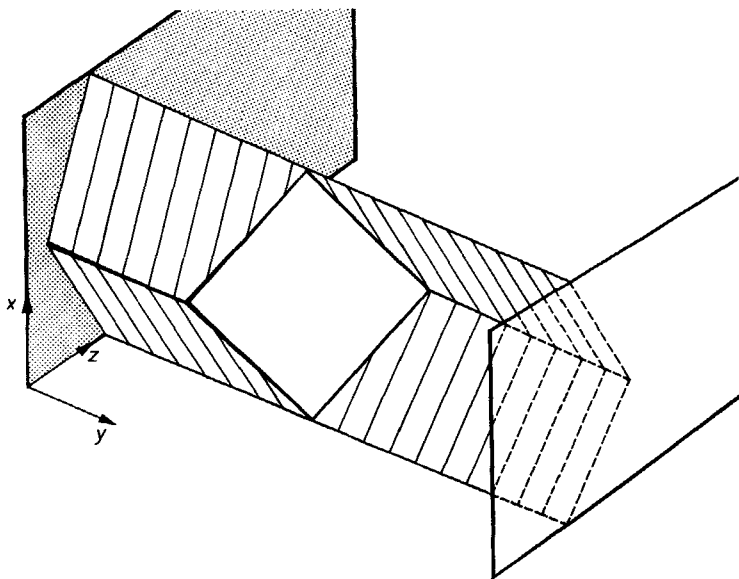

Figure 7.   In the recent literature ([10, 11]) authors mention two dimensional structures, as illustrated in this figure.

describing the inclination along the x-axis and y-axis respectively. The direction coefficients of the normal to the surface are $(-u, -v, 1)$ (unnormalized), so that, if the distance in the z-direction between layers is d_z, the perpendicular distance is

$$d_\perp = \frac{d_z}{\sqrt{(1+u^2+v^2)}} = l\cos\theta, \tag{25}$$

which determines the cone angle. The cone angle energy can therefore be expressed as a function of $1+u^2+v^2$

$$T\sin^2(\theta-\theta_c) = g(1+u^2+v^2). \tag{26}$$

The energy associated with the curvature of the layers can be described with some 'Oseen–Frank-like' expression of the normal vector $(-u, -v, 1)$. Since the divergence of this vector is $-\partial u/\partial x - \partial v/\partial y$ and since its curl is zero, this expression is

$$A\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)^2, \tag{27}$$

and the total 'positional energy' can be written as

$$\int L(u, v, u_x, v_y)\,dx\,dy, \tag{28}$$

with

$$L = A\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)^2 + g(1+u^2+v^2). \tag{29}$$

The Euler–Lagrange equations for the optimal form of the layers

$$\left.\begin{aligned}
\frac{\partial L}{\partial u}-\frac{\partial}{\partial x}\frac{\partial L}{\partial u_x}&=0, \\[2mm]
\frac{\partial L}{\partial v}-\frac{\partial}{\partial y}\frac{\partial L}{\partial v_y}&=0,
\end{aligned}\right\} \tag{30}$$

reduce to

$$\left.\begin{aligned}
A\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)&=g'u, \\[2mm]
A\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)&=g'v,
\end{aligned}\right\} \tag{31}$$

where g' denotes the derivative of the function g towards its argument $(1+u^2+v^2)$. A general solution of these equations, taking the boundary conditions ($u=0, v=u_e$ on the left side of the tip and $u=-u_e, v=0$ on the right side of the tip, see figure 8), could not be found.

If however, we use the same approximation as in §3, i.e. consider the cone angle energy to be constant in the chevron tip
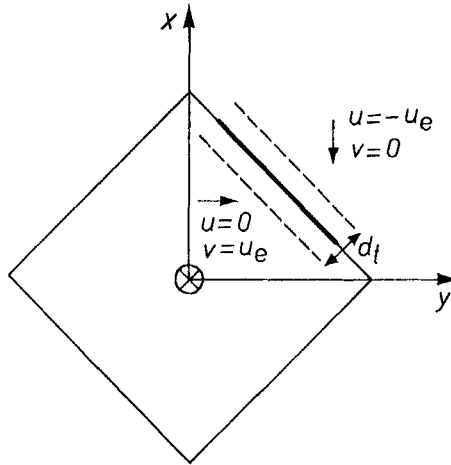
$$g = g_m \tag{32}$$

Figure 8. The boundary conditions at the border of the diamond-shaped surface in the more complicated structures as seen in figure 7.

then equation (31) shows that in the tip

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = \text{constant}$$

$$= -\frac{2u_e}{d_t\sqrt{2}}, \tag{33}$$

so that u goes linearly from 0 to $-u_e$ and v likewise from u_e to 0. The optimal thickness of the tip can then easily be calculated. One has per unit length of the tip

$$\gamma = A\frac{2u_e^2}{d_t^2}d_t + g_m d_t, \tag{34}$$

which is minimal for

$$d_t = \sqrt{\left(\frac{2A}{g_m}\right)}u_e, \tag{35}$$

and has then the value

$$\gamma_{\min} = 2\sqrt{(2Ag_m)}\,u_e. \tag{36}$$

In calculating this optimal form of the chevron tip, we have not taken account of the Oseen–Frank energy of the molecules and the electrostatic free energy. Even for the two states where the molecules are parallel to the glass surface, the molecules are not parallel to each other at both sides of the chevron tip, and thus *a fortiori* not through the tip. Moreover, there is a jump in the normal component of the polarization through the tip, and thus polarization charge density on the tip. These effects have not been taken into account. We think that an extension of the exact computer analysis, as presented for the one dimensional case in § 4, towards the two dimensional situation is practically not feasible. However, we think that it is reasonable to assume that the tip is infinitely small, and that the Frank–Oseen energy is proportional to $\sin^2\psi$ where ψ is the angle between the director at each side of the tip. With this assumption, an exact computer analysis of these two dimensional layer structures should be possible.

6. Conclusion

In this article we analysed the important factors which govern the tip width of one dimensional chevrons and the analogous width of 'fracture lines' in two dimensional structures. We indicated that the competition between two energy contributions is crucial: first the deviation of the layers from the planar structure and secondly the deviation of the smectic cone angle from its equilibrium value. Since the layers are fixed at the boundaries, nature has to look for a compromise. The influence of an applied electric field can only be numerically studied. Our computer program shows that slight layer bending can occur only if one assumes high compressibility.

Further investigation is needed. The full energy expression, equation (3) should be used. Finer estimations of the energy parameters of the electrical energy in two dimensional models would be a further improvement.

Appendix

In §3, the expression

$$\gamma = \int L(\delta, \dot{\delta})\, dx$$

$$= \int \left[A\left(\frac{d\delta}{dx}\right)^2 + g(\delta) \right] dx, \tag{37}$$

has to be minimized. The Euler–Lagrange equation

$$\frac{\partial L}{\partial \delta} - \frac{d}{dx}\frac{\partial L}{\partial \dot{\delta}} = 0 \tag{38}$$

reduces to

$$\frac{dg}{d\delta} - \frac{d}{dx}\left[2A\frac{d\delta}{dx} \right] = 0. \tag{39}$$

After multiplication with $d\delta/dx$, one obtains

$$\frac{dg}{dx} = \frac{d}{dx} A\left(\frac{d\delta}{dx}\right)^2. \tag{40}$$

Taking the boundary conditions at the glass surface into account $(\delta = \delta_e,\, g(\delta_e) = 0)$, one obtains

$$A\left(\frac{d\delta}{dx}\right)^2 = g(\delta). \tag{41}$$

The minimum value of γ is then

$$\gamma = 2 \int g(\delta)\, dx$$

$$= 2 \int g(\delta)\frac{1}{(d\delta/dx)}\, d\delta$$

$$= 2\sqrt{A} \int \sqrt{[g(\delta)]}\, d\delta, \tag{42}$$

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