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Director reorientation dynamics in chevron ferroelectric liquid crystal cells

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We present sample numerical solutions of the equation of motion that governs the dynamics of molecular orientation in ferroelectric liquid crystal cells with chevron layer structure. We show that the chevron structure significantly influences the director field, the chevron interface providing surface stabilization on a plane interior to the FLC layer. Assuming non-polar nematic-like elasticity in the vicinity of the chevron interface, we have modelled the effects of applied field on cells with purely non-polar cell boundary interactions that have uniform director orientation at zero field, and on cells in which the cell walls are strongly polar and the zero-field states are splayed. The simulations with strongly polar surfaces give bistable operation with the two states having fixed orientations at the FLC-solid surfaces, different orientation of **P** at the chevron interface, and **P** splayed in either the upper or lower portion of the cell. A monostable state can arise when the chevron interface is asymmetric, i.e. located away from the middle of the cell. Experimental results on asymmetric chevron cells qualitatively confirm the calculated switching scenario.

1. Introduction

The spatial variation of the director ($\hat{n}$) and polarization (**P**) fields of surface stabilized ferroelectric liquid crystals (SSFLCs) is determined both by coupling to external fields, as well as by interactions at various planar interfaces, both bounding and internal to the FLC. Knowledge of these surface interactions is of central importance in understanding the physics of director reorientation in FLC cells and in designing electro-optic devices. Handschy *et al.* [1] developed a theory which, through numerical simulations assuming uniform smectic layering in the bookshelf geometry, allowed the prediction of such quantities as the number of stable states in the absence of applied field (and their molecular orientation configuration), the critical values of electric field required for changes of state (reorientation transitions), and the optical properties of the device for a given electric field [2, 3]. Recent X-ray experiments by Rieker *et al.* [4] have since revealed that many SSFLC cells prepared with planar boundary conditions (molecules parallel to the bounding plates) do not have uniformly planar layering, but rather that the smectic layers exist in a chevron shaped (> > > > >) geometry (figure 1). The layers are uniformly tilted, in opposite senses, above and below a narrow, planar interface often situated about midway between the

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bounding plates. The experiments suggest that the chevron interface is extremely sharp, and that the region of layer bend can effectively be regarded as a surface [5]. The discovery of the chevron structure, when combined with the relationship of pretilt to layer tilt proposed by Handschy and Clark [1], leads naturally to the pretilt condition proposed by Ouchi *et al.* to explain the existence of the internal disclination [6] found to mediate the director reorientation.

Many of the director reorientation phenomena of chevron cells can be obtained by analogy with those found in cells with uniform layering, and we have not sought to repeat in detail the kinds of calculations done by Handschy and Clark. Instead we present the results of only a few simulations, namely director reorientation in a uniform cell and in a splayed cell, that typify chevron cells. We show that any quantitative understanding of the director-polarization structure in chevron cells requires consideration of all the following: (1) the interaction (surface stabilization) of the director at the chevron interface; (2) surface stabilization of the director at the FLC-solid surfaces, via polar and nonpolar interactions; (3) the resulting nonuniformity of the $\hat{n}$-**P** field.

2. Surface energies

Surface effects of relevance to SSFLC devices can be classified as either *homogeneous*, arising from the interaction of the LC with a spatially uniform interface, or *inhomogeneous*, resulting from localized defects (like dust or chemical differences on a bounding plate). Surface inhomogeneities *are* important in FLC devices, since they can nucleate switched surface domains at a lower field than would otherwise be expected. These domains can then grow by the motion of two- or three-dimensional domain walls, which propagate along the surface until they meet other walls and coalesce with them, at which time the entire surface has been switched [7]. We confine the present discussion to the effects of homogeneous surface interactions, which can be characterized by a surface energy per unit area that depends on the molecular orientation at the surface. These include LC-surface interactions at uniformly prepared bounding plates, as well as the LC–LC interactions at the chevron interface. In addition, we assume that ϕ is a function of x only. A one-dimensional model is applicable only in the absence of surface domain walls, a condition which can be achieved either by slowly varying the applied field in voltage regimes far from those at which surface domains are nucleated, or in the case of high voltage switching, when the surfaces reorient everywhere at the same time (i.e. homogeneously) without forming surface domains [1, 7].

At the bounding plates, we introduce non-polar interaction energy similar to that used to describe nematics, of the form $W_1 = -\gamma_1(\cos\psi)^2$, where ψ is the angle between $\hat{n}$ and the surface of the plate. $\gamma_1 > 0$ thus favours director orientation parallel to the bounding plates (planar alignment). As originally pointed out by Handschy *et al.* [3], the symmetry of FLCs requires, in addition a *polar* surface interaction that distinguishes between molecular orientations that differ in the sign of $\mathbf{P} \cdot \hat{s}$, where $\hat{s}$ is the surface normal unit vector pointing out of the FLC material. This results in an additional surface energy term of the form $W_2 = -\gamma_2(\hat{P} \cdot \hat{s})$. If γ_2 is sufficiently large compared with γ_1, then the state of lowest energy at zero applied field is a non-uniform or splayed state. In the simplest case, application of a sufficiently large electric field can reorient the surfaces and force the system into a more uniform configuration but if the field is subsequently removed, the system relaxes back to

being splayed. The relative stability of the splayed and uniform states depends on the field strength and surface energies in a non-trivial way [1].

The energy of the internal chevron interface is determined by the angular discontinuity in the director field, $\chi(\phi_+, \phi_-)$, where ϕ_+ and ϕ_- are respectively the dipole orientations just above and just below the chevron interface, and ϕ is in general the angle between **P** and the in-layer component ($E_x \cos\delta$) of the external electric field, where δ is the layer tilt angle.

Since in most cases the director tilt angle θ is comparable to δ ($\theta \gtrsim \delta$), we have $\chi \ll 1$ and can assume a simple interface energy of the form $W_4 = -\gamma_4 \cos\chi$, which is minimized ($\propto \chi^2$) when the directors $\hat{n}_+$ and $\hat{n}_-$ are parallel ($\chi = 0$). This nematic-like binding energy does not explicity account for the effect of space charges at the chevron interface which result from a discontinuity in the normal component of **P**. Of course, a non-zero divergence of **P** *anywhere* in the sample leads to the appearance of bound charge and a resultant alteration of the local E field [9], so it would clearly be desirable to include these effects in the model in general. This will be treated in a later publication [10].

3. Equations of motion

The equations of motion are derived by minimizing the total free energy of the FLC plus surfaces system. We begin with the surface energies, assuming that the smectic layers are tilted by $\pm\delta$ respectively above and below the chevron interface (as in figure 1) and that the FLC molecules have positive polarization, i.e. that $+\hat{P}\sin\theta = \hat{z} \times \hat{n}$, where θ is the usual Smectic C (SC) tilt angle. The elevation angle ψ between the director $\hat{n}$ and the bounding plates is given by

$$\cos^2\psi = \cos^2\delta\cos^2\theta + \sin^2\theta - \cos^2\delta\sin^2\theta\sin^2\phi \pm \tfrac{1}{2}\sin 2\theta \sin 2\delta \sin\phi,$$

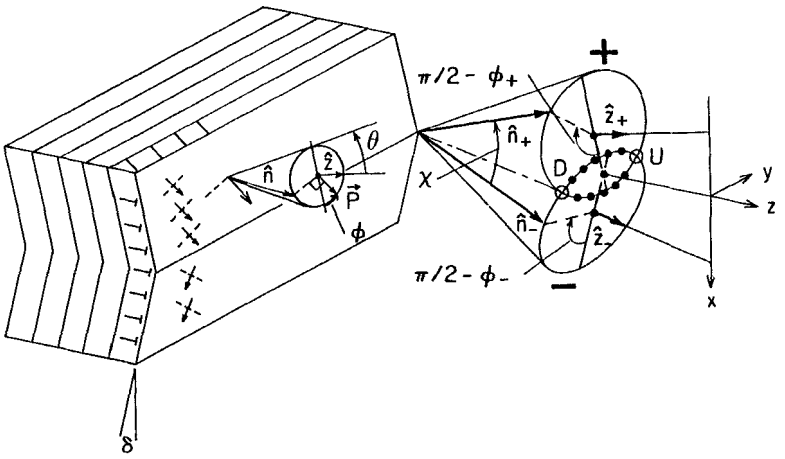

Figure 1. Geometry of the director field at a Smectic C chevron: The SC is a locally biaxial structure of liquid-like layers in which $\hat{n}(r)$ is tilted at an equilibrium angle θ relative to the local layer normal $\hat{z}_+(r)$ or $\hat{z}_-(r)$ and is free to reorient azimuthally through the angle ϕ on a cone of axis $\hat{z}_+$ (or $\hat{z}_-$). Subscripts + and − refer to quantities on opposite sides of the chevron. For $\delta < \theta$, the cone intersections U and D (open circles) are the equilibirum orientation of $\hat{n}$, having $\hat{n}$ parallel to the interface. In these states the FLC polarization **P** is pretilted such that starting from the D state and applying a field **E** along $\hat{x}$, the polarizations rotate in opposite directions on opposite sides of the chevron, moving along the dotted paths from D to U for sufficiently large E. Reproduced from [5].

where the $\pm$ signs refer to the top and bottom plates respectively. The component of the polarization **P** normal to the bounding plates is $P_x = P\cos\phi\cos\delta$. The bounding surface energy terms can then be combined as

$$W_s = -\gamma_1(\cos\psi)^2 - \gamma_2\left(\frac{\hat{x}\cdot\hat{s}}{|\hat{x}\cdot\hat{s}|}\right)\cos\phi\cos\delta. \tag{1}$$

At the chevron interface, the tilt cones defining the allowed director orientations above and below the interface intersect in general in two places (see figure 1). The angle χ between the directors above and below the interface is given implicitly by

$$\begin{aligned}\cos\chi = {} & \cos 2\delta\cos^2\theta + \sin 2\delta\sin\theta\cos\theta(\sin\phi_+ - \sin\phi_-) \\ & + \cos 2\delta\sin^2\theta\sin\phi_+\sin\phi_- + \sin^2\theta\cos\phi_+\cos\phi_-\end{aligned}$$

and the corresponding surface energy by

$$W_s = -\gamma_4\cos\chi. \tag{2}$$

To obtain a completely uniform cell of the lowest possible energy with $\gamma_1, \gamma_4 > 0$ and $\gamma_2 = 0$, the directors are required to be parallel to very interface as well as to each other throughout the cell. This uniform director orientation is achieved at the expense of a discontinuity in P_y, the component of **P** parallel to the interfaces, which changes sign at the chevron interface. The resultant configuration obeys the relation

$$\sin\phi = \pm\frac{\tan\delta}{\tan\theta},$$

where the $\pm$ signs refer to the orientation ϕ in the upper and lower parts of the cell as usual.

It is clear that layer tilt combined with surface energies of the kind we have described always results in some zero-field 'pretilt' of the ferroelectric polarization at the various interfaces, i.e. P_y (or $\sin\phi$) is in general non-zero at the surfaces. The amount of pretilt depends on the layer tilt $\pm\delta$ and on the strength (and sign) of the surface interactions. The discovery of the chevron structure thus provides *a posteriori* justification for the asymmetric polarization pretilt previously assumed by Fukuda's group (see, for example, [11]) in order to explain observations of director reorientation in FLC cells using models with uniformly planar layering, since it automatically assures pretilt of opposite sign at the bounding plates.

The total electrostatic + distortion free energy of the system can be written, using the one-elastic-constant approximation, as

$$\begin{aligned}F = {} & \int_{-d/2}^{d/2}\frac{K}{2}\phi_x^2 - PE\cos\phi + Kq_s\sin\phi\phi_x dx \\ & -\gamma_1(\cos^2\psi_b + \cos^2\psi_t) - \gamma_2\cos\delta(\cos\phi_t - \cos\phi_b) - \gamma_4\cos\chi,\end{aligned} \tag{3}$$

where the γ_i are surface energy anisotropies per unit area, q_s is the wavevector characteristic of the spontaneous splay of the polarization [1], and we have ignored any dielectric or flexoelectric contributions. The subscripts b and t refer to the bottom and top of the cell.

Scaling x by the cell thickness d gives

$$\frac{Fd^2}{K} = \int_{-1/2}^{1/2} \phi_x^2 - \lambda_3^2 \cos\phi dx$$
$$- \lambda_1(\cos^2\psi_b + \cos^2\psi_t) + \lambda_2 \cos\delta(\cos\phi_t - \cos\phi_b) - \lambda_4 \cos\chi, \quad (4)$$

where $\lambda_1 = \gamma_1 d/K$, $\lambda_2 = (q_s + \gamma_2/K)d$, $\lambda_4 = \gamma_4 d/K$, and $\lambda_3 = d(PE/K)^{1/2} = d/\xi$, where $\xi = (K/PE)^{1/2}$ defines the electric field correlation length.

The equilibrium state that minimizes this free energy satisfies simultaneously the Euler–Lagrange equation

$$\phi_{xx} = \lambda_3^2 \sin\phi,$$

and a surface torque balance equation at each interface, of the form

$$\pm \left.\frac{\partial f}{\partial \phi_x}\right|_s + \left.\frac{\partial W}{\partial \phi_x}\right|_s = 0,$$

where this equation must effectively be applied twice at the chevron interface, once to constrain ϕ_- and once to constrain ϕ_+. If we add a term to describe viscous damping of the director reorientation on the tilt cone, we get the dynamic equation

$$\partial\phi/\partial t = \phi_{xx} - \lambda_3^2 \sin\phi, \quad (5)$$

which has time t in units of $\eta d^2/K = \lambda_3^2 \tau$, where $\tau = \eta/PE$ is the characteristic time for director reorientation in a uniformly oriented sample.

4. Simulations of director reorientation dynamics

We solved equation (5) numerically for various surface strength parameters and different field strengths using computational techniques we have described in an earlier paper [12]. We assumed that the bounding plates were identical, i.e. that λ_1 and λ_2 were the same on both plates. We measured the temporal evolution of these systems under the influence of electric field reversal, as well as obtaining the equilibirum states at different d.c. field strengths. In every simulation, $\theta = 22°$ and $\delta = \pm 18°$ these numbers being typical of the configurations found in the X-ray experiments. We assumed, to begin with, that the chevron interface was located in the middle of the cell.

4.1. *Uniform cell*

In the absence of polar surface interactions, the FLC adopts a uniform orientation at zero applied field, as shown in figure 2. The chosen surface strength parameters ($\lambda_1 = 200, \lambda_2 = 0, \lambda_4 = 440$) stabilize two energetically-equivalent, pretilted uniform states, UP ($\phi \approx 2\pi/3$ above the chevron interface and $\phi \approx -2\pi/3$ below the chevron interface) and DOWN ($\phi \approx \pi/3$ above the chevron interface and $\phi \approx -\pi/3$ below the chevron interface). Figure 2 (*a*) illustrates the dynamics of director reorientation in this cell. The initial DOWN field (of stength $\lambda_3 = 8$) is reversed at $t = 0$ and the system then evolves to the final equilibrium UP state. Figure 2 (*b*) shows the distorted states that are stable in strong UP and DOWN fields respectively, and the uniform states to which they relax when the applied field is removed. Figure 2 (*c*) shows the result of slowly varying the applied field from $\lambda_3 = +8$ to $\lambda_3 = -8$. The system starts off in the DOWN state and, as the field strength is reduced through zero,

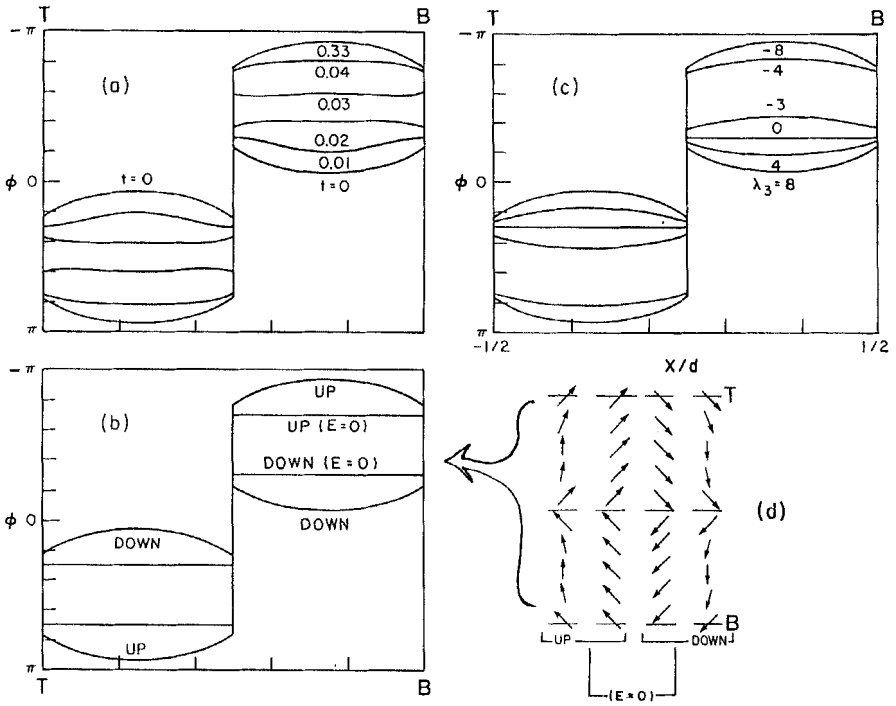

Figure 2. Director reorientation in a uniform chevron cell vs. x/d (= $+1/2$ at the BOTTOM, = $-1/2$ at the TOP). (*a*) stages in the evolution from DOWN to UP after an applied field reversal; times are in units of $\eta d^2/K$; (*b*) stable states in UP and DOWN fields and the uniform states these relax to when the field is removed ($E = 0$); (*c*) equilibrium director orientation as a function of applied field. The field strength is slowly varied from $\lambda_3 = +8$ to $\lambda_3 = -8$ and the samples switches from mostly DOWN to mostly UP at a threshold of $\lambda_3 \approx -3$. The surface strength parameters are $\lambda_1 = 200$, $\lambda_2 = 0$ and $\lambda_4 = 440$. (*d*) geometry of **P** in the four states in (*b*).

reorients continuously towards the UP state. At a threshold field of $\lambda_3 \approx -3$, the surface energy barriers can be overcome and the polarization switches discontinuously to UP. This is a first order orientational transition of the kind first proposed by Handschy *et al.* [3] and recently confirmed experimentally by Xue *et al.* [13]. Figure 2(*d*) shows the geometry of the four states of figure 2(*b*).

4.2. *Splayed cell*

With a polar surface energy $\lambda_2 = +11$, which favours the orientations $\phi_t = 0$ and $\phi_b = \pi$, the zero-field equilbrium director orientation is non-uniform, as shown in figure 3. The other surface strength parameters are the same as before and combine with the polar term to stabilize two different (but symmetric and energetically equivalent) splayed polarization states at zero field. Figure 3(*a*) shows the evolution of this splayed system subsequent to a field reversal. Figure 3(*b*) shows the equilibrium states in UP and DOWN fields respectively, and the splayed states to which they relax when the applied field is removed. As in the uniform case of figure 2(*b*), this system exhibits bistability, the UP state relaxing to a configuration which has most of its splay *below* the chevron, while DOWN relaxes to a state which is more splayed *above* the chevron. In figure 3(*c*) we show the result of slowly varying

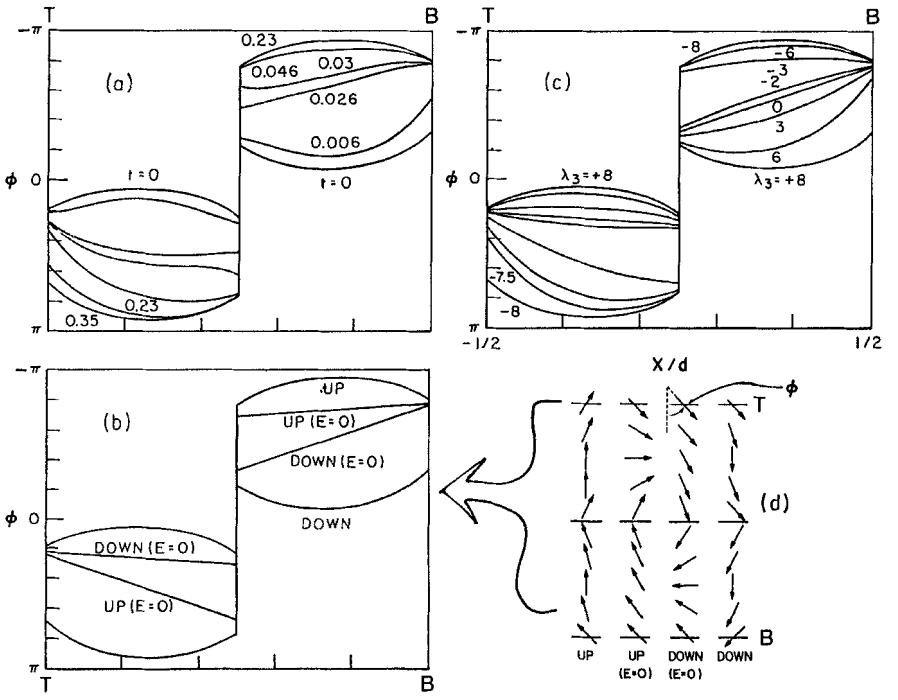

Figure 3. Director reorientation in a splayed chevron cell vs. x/d ($= +1/2$ at the BOTTOM, $-1/2$ at the TOP). (*a*) stages in the evolution from DOWN to UP after an applied field reversal (*b*) equilibrium states in UP and DOWN fields and the splayed states these relax to when the field is removed ($E = 0$); (*c*) equilibrium director orientation as a function of applied field. The field strength is slowly varied from $\lambda_3 = -+8$ to $\lambda_3 = -8$. The directors at the chevron switch at $\lambda_3 \approx -2{\cdot}5$, at which point the sample becomes predominantly UP. The region near the lower cell surface switches only at a higher field, $\lambda_3 \approx -7{\cdot}5$. The surface strength parameters are $\lambda_1 = 200$, $\lambda_2 = +11$ and $\lambda_4 = 440$, (*d*) geometry of P in the four states in (*b*).

the applied field from $\lambda_3 = +8$ to $\lambda_3 = -8$. Here we can distinguish *two* well-defined threshold fields. For $\lambda_3 \approx -2{\cdot}5$ there is an abrupt reorientation transition at the chevron interface. At an even higher field ($\lambda_3 \approx -7{\cdot}5$) the polarization at the lower bounding plate can also be switched to UP, although in our example λ_1/λ_2 is too small to latch the surface in this state. Figure 3 (*d*) shows the geometry of **P** for the states in figure 3 (*b*). The UP and DOWN states differ in orientation at the chevron interface. These are stabilized states, separated by a first order transition. If both states are present at a given time, there will be sharp domain walls separating the UP and DOWN chevron surface domains. These domain walls will typically have the characteristic 'boat' slope [6], shown in figure 5.

4.3. *Asymmetric chevron*

In a splayed cell with the chevron interface displaced from the cell centre, the UP and DOWN states are of different total energy, the state having the splay in the wider portion having lower energy if $q_s = 0$. In general the states will be 'stabilized', i.e. there will be a stable and a metastable state separated by an energy maximum. However, chevron interface is located sufficiently far from the middle, the maximum in the energy vs ϕ at the chevron interface will disappear and the cell will become

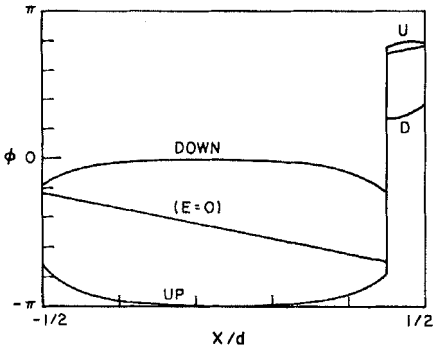

Figure 4. Monostability in a splayed, asymmetric chevron cell. With the chevron situated 90 per cent of the way from one of the bounding plates, the equilibrium states in UP and DOWN fields both relax to the same splayed state when the field is removed. The surface strength parameters are $\lambda_1 = 200$, $\lambda_2 = +11$ and $\lambda_4 = 440$.

monostable, the director field relaxing without domain walls in the absence of applied electric field to a state which minimizes the splay in the upper (narrower) part of the chevron, as shown in figure 4. The particular orientation stabilized at the chevron will depend on the orientation of **P** preferred at the solid-FLC surfaces. Using the same surface energies as in the previous example requires that the interface be moved at least 90 per cent of the way to one of the bounding plates for this effect to occur but with different parameters one should be able to get monostability with a less asymmetric chevron.

In a bistable splayed asymmetric chevron cell with a stable and metastable state of $\hat{n}$-**P** at the chevron, the switching threshold will be no longer symmetric about $V = 0$. This is shown directly in figure 5, photomicrographs of an asymmetric chevron cell with zig-zag walls. As the zig-zag wall is crossed, the chevron interface location is reflected through the cell midplane, switching from the lower half (dark) to the upper half (bright) of the cell (or vice versa) [5, 14]. At the DC applied voltage $V_a = 0$, the orientation at the chevron interface is UP in the dark region and DOWN in the light region, as indicated in figure 5 (*b*). As the applied DC voltage is increased from 0 the UP → DOWN boat shaped reorientation domains, known to be associated with the two stabilized states of $\hat{n}$-**P** at the chevron interface [5, 14] appear only on one side of the zig-zag (*at* +0·8 V, figure 5 (*c*)), $\hat{n}$-**P** already being DOWN on the other side of the zigzag wall. However, chevron surface domains do appear in the $V_a = 0$ DOWN region when a negative voltage is applied ($V_a = -0{\cdot}7$ V, figure 5 (*b*)). This observation provides evidence for the asymmetry of the chevron interface positions and its displacement upon crossing a zig-zag wall and, by inference, for the orientation constraint at the chevron interface [14] and the polarization distributions illustrated in figure 5.

5. Conclusion

Experimental observations indicate that the chevron structure is the rule in SSFLC cells prepared with second order smectic A to smectic C materials and planar boundary conditions. The inclusion of an internal interface characterized by a finite orientational surface energy introduces a fundamental new aspect to the physics of the orientation field in such cells. Our model shows the existence of orientation states, stabilized by the chevron interface, which may be uniform on one side of the chevron

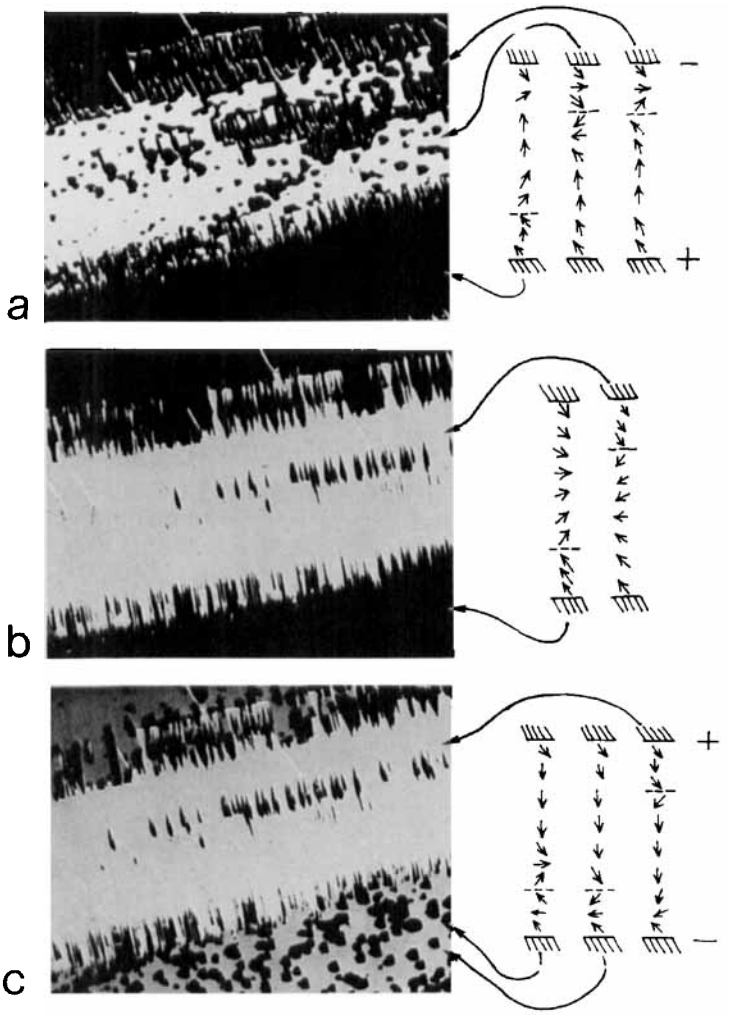

Figure 5. (*a*) Field induced chevron surface domains [14] in a Chisso 1014 asymmetric chevron cell having zig-zag walls (rubbed nylon alignment). (*b*) at $V = 0$ bands of zig-zag walls run horizontally along the cell, dividing regions where the chevron interface is in the upper half (toward the reader), bright in (*b*)) from regions where the chevron interface is in the lower half (dark in (*b*)). The UP state (dark) is preferred where the chevron interface is in the lower half. (*a*) $V = -0{\cdot}7\ V$ on the TOP electrode, near the DOWN → UP chevron interface switching threshold in the cell portion having the chevron interface in the upper half. **P** at the chevron interface is completely UP, there the chevron interface is in the lower half. (*c*) $V = +0{\cdot}8\ V$ on the top electrode, near the UP → DOWN chevron interface switching threshold in the cell portion having the chevron interface in the lower half. The drawings show the distributions of **P** in the indicated portions of the cell.

and splayed on the other (generally the rule near $V_a = 0$ with second order A–C materials and planar boundary conditions), and are either mono- or bistable. Finally, we point out that the electro-optic response of chevron cells can be calculated directly from the results of our simulations [15], and that to quantitatively understand the optics, the influence of the chevron interface on the director field must be included. Photomicrogaphs of chevron interface domain mediated switching in a splayed asymmetric chevron cell with zig-zag walls confirms the overall picture presented in the calculations.

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