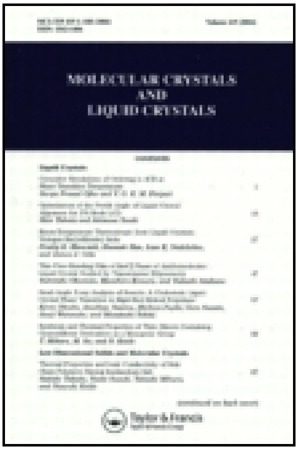

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The Influence of Polar Surface Anchoring on Switching in Antiferroelectric Liquid Crystals

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The Influence of Polar Surface Anchoring on Switching in Antiferroelectric Liquid Crystals

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We present a theoretical investigation into the effects of polar anchoring in a liquid crystal cell containing an antiferroelectric liquid crystalline material. Our model includes effects due to finite polar and non-polar anchoring, quadrupolar ordering and polarization self interaction. We find that the presence of quadrupolar ordering or weak anchoring means that the cell may be *primed* into the thresholdless state through a discontinuous transition from an initial antiferroelectric state.

Keywords: antiferroelectric liquid crystals; polar anchoring; theory; thresholdless switching; quadrupolar ordering

INTRODUCTION

Recently there has been an increased interest in thresholdless modes of operation of AFLC cells [1,2]. In such cells the material continuously transforms from the antiferroelectric (AF) state to either of the ferroelectric (F) states upon application of an electric field. In liquid crystal devices such thresholdless switching modes have been of significant scientific and technological interest for some time. In nematic devices the Hybrid Aligned Nematic cell [3,4] and the π-cell [5] are operated in a thresholdless mode whilst for smectic devices the ferroelectric liquid crystal (FLC) deformed helix [6] and twisted FLC devices [7,8] and antiferroelectric liquid crystal (AFLC) materials [9] all exhibit thresholdless switching.

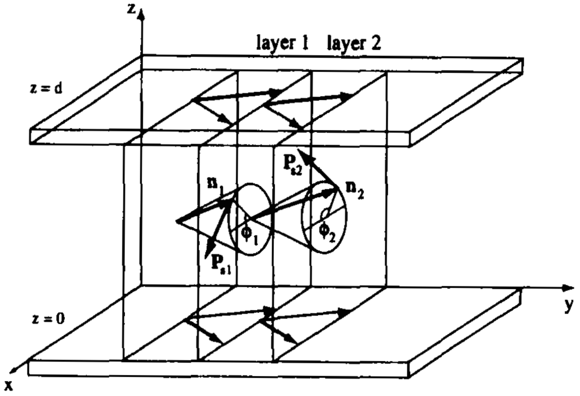

Figure 1: Cell configuration: The directors, $\mathbf{n}_1$ and $\mathbf{n}_2$, in layers 1 and 2 respectively lie on the smectic cone while the corresponding polarization vectors $\mathbf{P}_{s1}$ and $\mathbf{P}_{s2}$ lie in the xz plane perpendicular to the directors. The layers are in the bookshelf configuration between glass plates at $z = 0$ and $z = d$. At the cell surfaces the polar anchored director state (dark arrows) is the globally stable state whilst the anti-polar anchored state (light arrows) is metastable.

The advantages of using AFLC materials (fast, in-plane, symmetric driving schemes and large contrast ratio) led researchers to investigate the possibility of obtaining a thresholdless AFLC mode. In an apparently antiferroelectric (AF) material Inui *et al* [9] observed a thresholdless mode which they explained in terms of a *random smectic* model where the director correlation between adjacent layers was small. However, recent experimental observations [1,2] suggest that a more realistic model for this behavior is a twisted smectic structure in which the AF ordering of the material is suppressed and the liquid crystal is in fact in the ferroelectric phase. In many situations the cell must first be *primed* into the thresholdless state [1,10] by applying an electric field. After the cell has been primed it switches thresholdlessly. However, when the field is removed and the cell remains in the zero voltage state for some time (which can be between hours and days) the *unprimed* ground state is recovered and the cell must first be primed again before thresholdless switching occurs. In this paper we present a model of an AFLC cell in order to investigate the effects of polar anchoring and find similar priming behaviour.

THE MODEL

The model used in this paper is an extension of our previous model [11] to include weak anchoring and quadrupolar ordering. We will assume that the smectic layers are in a bookshelf configuration and that the director within each layer lies on the smectic cone with a fixed cone angle (see Fig. 1). We also assume that the behavior may be modeled by only considering two adjacent smectic layers. This is equivalent to assuming that there is no helix present in the cell and thus the material is surface stabilized.

At the cell boundary plates ($z = 0, d$) the molecules prefer to lie on the cell surface rather than parallel to it. In other words the director would like to lie on either side of the smectic cone ($\phi = 0$ or π). However since the materials which we are attempting to model have a high molecular spontaneous polarization ($|\mathbf{P}_s| \approx 5 \times 10^{-4} - 1 \times 10^{-3}\mathrm{C/m^2}$) there will be a strong interaction between the surface alignment layer and the permanent molecular dipole. Thus the surfaces induce polar anchoring and the global surface energy minima is $\phi = 0$ at $z = 0$ and $\phi = \pi$ at $z = d$ whilst the other states are metastable minima. Such boundary conditions prefer the material to be in the ferroelectric phase at the surfaces.

If the director in each layer remains on a cone of angle θ and the layers are in the bookshelf configuration then we can write $\mathbf{n}_i = (\sin\theta\cos\phi_i, \cos\theta, \sin\theta\sin\phi_i)$ where $i = 1, 2$ indicates the first or second layer and ϕ_i is the azimuthal director angle around the smectic cone. The corresponding spontaneous polarization vectors which lie perpendicular to $\mathbf{n}_i$ and the y axis are then $\mathbf{P}_{si} =$

$P_s\left(\sin\phi_i,\ 0,\ -\cos\phi_i\right)$. The free energy may be written as,

$$\begin{aligned}
\mathcal{F} \;=\; & \frac{\epsilon_0 V^2}{2d\int_0^1 \frac{1}{\epsilon_{zz}}dZ} - \frac{V\int_0^1 \frac{P_z}{\epsilon_{zz}}dZ}{\int_0^1 \frac{1}{\epsilon_{zz}}dZ} + \frac{d\left(\int_0^1 \frac{P_z}{\epsilon_{zz}}dZ\right)^2}{2\epsilon_0\int_0^1 \frac{1}{\epsilon_{zz}}dZ} - \frac{d}{2\epsilon_0}\int_0^1 \frac{P_z{}^2}{\epsilon_{zz}}dZ \\
& + \frac{K\sin^2\theta}{2d}\int_0^1 \left(\left(\frac{d\phi_1}{dZ}\right)^2 + \left(\frac{d\phi_2}{dZ}\right)^2\right)dZ \\
& + \gamma d\int_0^1 \cos\left(\phi_1-\phi_2\right)dZ - \gamma_q d\int_0^1 \cos^2\left(\phi_1-\phi_2\right)dZ \\
& + W_{np}\Big(\sin^2\left(\phi_1(0)\right) + \sin^2\left(\phi_2(0)\right) \\
& \qquad + \sin^2\left(\phi_1(1)\right) + \sin^2\left(\phi_2(1)\right)\Big) \\
& + W_p\left(\sin^2\left(\phi_1(0)/2\right) + \sin^2\left(\phi_2(0)/2\right)\right) \\
& + W_p\left(\cos^2\left(\phi_1(1)/2\right) + \cos^2\left(\phi_2(1)/2\right)\right), \qquad (1)
\end{aligned}$$

where $P_z = -P_s\left(\cos\phi_1 + \cos\phi_2\right)/2$ is the average polarization in the z direction and $\epsilon_{zz} = \epsilon_\perp + \Delta\epsilon\sin^2\theta\left(\sin^2\phi_1 + \sin^2\phi_2\right)/2$ is the average zz component of the dielectric tensor. In Eq. (1) the z coordinate has been nondimensionalised with the cell gap width d so that $Z = z/d$, V is the voltage applied across the cell, $\epsilon_0 = 8.85\times10^{-12}\mathrm{F/m}$ is the permitivity of free space, K is a Frank elastic constant, γ is the antiferroelectric ordering parameter, γ_q is the quadrupolar ordering parameter, W_{np} is the non-polar anchoring strength and W_p is the polar anchoring strength.

The first four terms in Eq. (1) describe the electrostatic energy contributions and are derived by solving Maxwell's equations [12] assuming that the electric properties may be averaged over the two layers. The fifth term is the elastic distortion energy which may be thought of as the Frank elastic energy (under a one constant approximation) of the nematic-like directors within each layer. The sixth and seventh terms describe the liquid crystal material's tendency to form ferro (F) or antiferroelectric (AF) states. When $\gamma > -2\gamma_q$ the AF state ($\phi_2 = \pi + \phi_1$) is stable in the bulk material and when $\gamma < 2\gamma_q$ the F state ($\phi_1 = \phi_2$) is stable. When both states are stable ($-2\gamma_q < \gamma < 2\gamma_q$) the AF state is the global energy minimum when $\gamma > 0$ and the F state when $\gamma < 0$. In this paper we will assume that we are below the smectic C - smectic C_A phase transition such that the F state is never the globally stable state but may be a metastable state. The last terms in Eq. (1) are surface energies and govern the behavior of the director close to the cell surfaces. The non-polar, W_{np} term describes the director's tendency to lie on the cell surfaces ($\phi_{1,2} = 0$ or π at $z = 0$ or d). The polar, W_p term describes the polar interaction between the surfaces and the director such that at $z = 0$ the directors prefer the orientation $\phi_{1,2} = 0$ and at $z = d$ the directors prefer $\phi_{1,2} = \pi$ as discussed in the previous section.

To investigate the dynamics of switching we use a relaxation technique which effectively solves the Ginzburg-Landau equation associated with the bulk energy in Eq. (1),

$$\mu\frac{\partial\phi_1}{\partial t} = -\mathcal{L}_{\phi_1}\left(F_{bulk}\right), \tag{2}$$

$$\mu\frac{\partial\phi_2}{\partial t} = -\mathcal{L}_{\phi_2}\left(F_{bulk}\right), \tag{3}$$

where F_{bulk} is the bulk free energy density associated with the non-surface energy terms in $\mathcal{F}$, $\mathcal{L}_u = \partial/\partial u - d(\partial/\partial u_Z)/dZ$ is the normal Lagrangian operator and μ is the viscosity of director motion around the smectic cone.

This theoretical model is clearly extremely complex. There are many independent parameters and although some may be fixed to values typical for AF materials (we set $\epsilon_\perp = 5.0$, $\Delta\epsilon = -1.5$, $\theta = 25°$, $P_s = 5 \times 10^{-4}\mathrm{C/m^2}$, $\mu = 100\mathrm{Ns/m}$ and $K = 10^{-11}\mathrm{N}$), we will want to alter other parameters in order to investigate the properties of the ground states and switching mechanism (i.e. the cell thickness, d, the ordering parameters γ and γ_q, which will be temperature dependent, the anchoring strengths, W_{np}, W_p and of course the applied voltage V). We have previously investigated the effects of altering the cell thickness and AF ordering when the surfaces induce strong polar anchoring to find the zero voltage ground states [11]. In the next section we will concentrate on two points in parameter space in order to investigate the switching behavior and priming effect of two thresholdless modes. These two sets of parameters typify the behavior of the system in large regions of parameter space and small changes in the parameters do not qualitatively change the switching behavior of the cell.

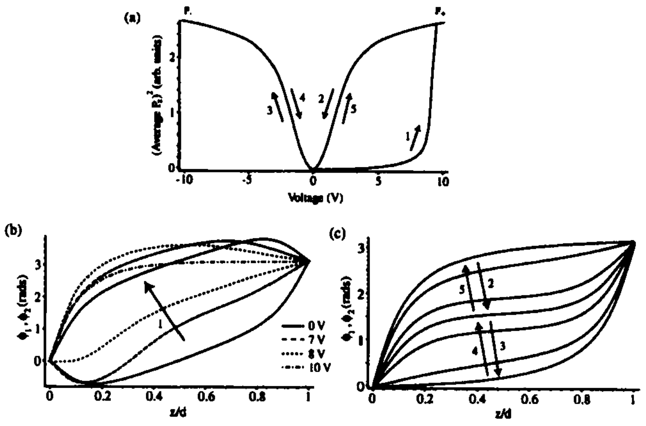

Figure 2: Priming to, and thresholdless switching of, the twisted smectic state. (a) The polarization in the z direction, averaged over the cell thickness, squared, versus voltage. (b) Initial switching from the AF state to the F state. (c) Thresholdless switching of the twisted smectic state where $\phi_1 = \phi_2$.

RESULTS

In a previous paper we found two director configurations could switch thresholdlessly, an F solution and an AF solution. The F solution was the twisted smectic state which has previously been invesitgated [7,8] and shown to swith thresholdlessly. In this configuration $\phi_1 = \phi_2$ and the material is in a ferroelectric smectic C state. We found that this state exists for low temperatures, since the material then prefers the F state, or when the cell thickness is small. This last case shows how the F ordering at the surfaces can influence the bulk behaviour of the cell. When d is small the behaviour at the surfaces dominates the bulk behaviour and the AF state is suppressed. In this paper we show how, due to the presence of quadrupolar ordering this F state may be stabilised, at least locally, within a temperature range at which the AF state is the lowest energy solution. The second thresholdless switching state was a vertical AF state, i.e. the directors are in the vertical yz plane so that $\phi_1 = \pi/2$ and $\phi_2 = 3\pi/2$. We have shown that this state may switch thresholdlessly in the absence of quadrupolar ordering. How ever in this AF state the directors in the two layers rotate in opposite directions through the cell and there was some doubt as to whether this state could be realised. In this paper we show how such a configuration may be achieved.

Firstly, we consider the twisted smectic C solution. In order to at least locally stabilize the F state at a low temperature a quadrupolar energy term must be introduced. The results are shown in Fig. 2. For this calculation we have used the parameter values $d = 10^{-6}$m, $\gamma = 10^3$N/m^2, $\gamma_q = 10^3$N/m^2 and assumed that there exists strong polar anchoring at the surfaces $W_{np} = 0$, $W_p \to \infty$ (i.e. the directors at the surface are fixed to be $\phi_{1,2}(0) = 0$ and $\phi_{1,2}(d) = \pi$). It should be noted that if the strong anchoring condition is relaxed such that W_p is finite but large, the switching behavior remains qualitatively the same.

In Fig. 2(a) we have plotted the average polarization in the z direction, squared, versus voltage to illustrate how the cell is first primed to the positive voltage F state (F$_+$) and then switches thresholdlessly between the F states (F$_+$ and F$_-$). As the field is initially increased the ground AF state switches hysteretically to the F$_+$ state [indicated by arrow 1 in Fig. 2(a)] with the director configuration switching from the ground state [solid lines in Fig. 2(b)] to the switched state [dash-dot lines in Fig. 2(b)]. From this point the F state is metastable, due to the presence of quadrupolar ordering, and will switch thresholdlessly in the same way as a twisted smectic device [7,8] [indicated by arrows 2-5 in Fig. 2(a)]. In the bulk of the cell the director azimuthal angle changes continuously from $\phi = \pi$ to $\phi = 0$ through the zero voltage ground state $\phi = \pi/2$ [Fig. 2(c)].

If the voltage is removed the F state remains but the system is in a high energy metastable state. If the system is perturbed (by surface defects, regions of AF ordering etc.) the system reverts to an AF ground state. We have confirmed this numerically by introducing a small numerical perturbation to allow the system to relax to the AF state. Once the system has relaxed to the ground state it will again

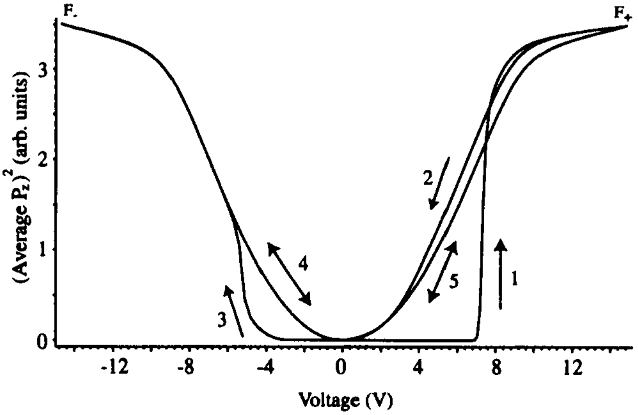

Figure 3: Priming to, and thresholdless switching of, the vertical AF state. The polarization in the z direction, averaged over the cell thickness, squared, versus voltage.

prime into an F state upon application of a voltage and then switch thresholdlessly. Such an effect would agree with the experimentally observed behavior previously mentioned.

The second situation we consider is priming into the vertical AF thresholdless state. We now demonstrate how this vertical AF state may be obtained from a uniform surface stabilized AF configuration. For this calculation we have used the parameter values $d = 10^{-6}$m, $\gamma = 10^3$N/m^2, $\gamma_q = 0$ so that there is no quadrupolar ordering and we assume that there is weak anchoring $W_{np} = 1.5 \times 10^{-4}$N/m, $W_p = 1.5 \times 10^{-4}$N/m which means the polar anchored state is the global energy minimizer with a metastable anti-polar state (see Fig. 1).

Figure 3 shows the response of the directors when, starting with a surface stabilized AF state ($\phi_1 = 0$, $\phi_2 = \pi$), a triangular voltage waveform is applied. Fig. 3 shows the average P_z response (squared) versus the applied voltage whilst Fig. 4 shows the director angle response when switching from $0V$ to $15V$ (a)-(d) on response branch 1 in Fig. 3, $15V$ to $0V$ (d)-(f) on response branch 2 in Fig. 3,

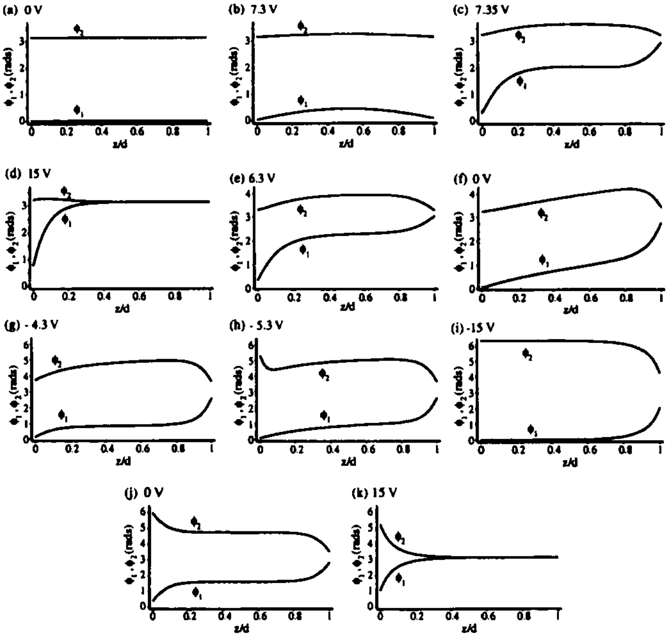

Figure 4: Solutions along the branches in Fig. 3

0V to -15V (f)-(i) on response branch 3 in Fig. 3 and finally Fig. 4(i)-(k) show the thresholdless response once the cell has been primed (on response branches 4 and 5 in Fig. 3).

Initially, when $V = 0$, the directors are in the AF state $\phi_1 = 0$, $\phi_2 = \pi$ [Fig. 4(a)]. At a critical voltage the bulk of the cell starts to switch to the F_+ state [Fig. 4(b)] and the surface anchoring at $z = d$ breaks [Fig. 4(c)] since the $\phi_1(d) = 0$ state is only metastable whilst the $\phi_1(d) = \pi$ state is globally stable. At the maximum field value most of the cell is in the F_+ state ($\phi_{1,2} = \pi$) except for the anchored region where $\phi_1(0)$ is much smaller than π [Fig. 4(d)].

As the voltage is then reduced to zero the directors relax to an AF state except near the anchored region at $z = d$ [Fig. 4(f)]. As the voltage further decreases to large negative values the directors move towards the F$_-$ state ($\phi_1 = 0$, $\phi_2 = 2\pi$) and the metastable anchoring, $\phi_2(0) = \pi$, breaks [see Figs. 4(g) and (h)] and switches to the globally stable position $\phi_2(0) = 2\pi$ [which is of course equivalent to $\phi_2(0) = 0$].

From then on the cell switches thresholdlessly between the two F states (with surface reorientation regions induced by the anchoring conditions). In the zero voltage ground state the bulk of the cell is in a vertical AF state, i.e. $\phi_1 = \pi/2$, $\phi_2 = 3\pi/2$ [Fig. 4(i-k)].

Thus there are two priming steps corresponding to the breaking of two surface anchoring conditions. It should be noted that for different parameter values, especially for smaller values of W_{np}, the second priming response may be very small.

As in the previous situation the *primed* zero voltage state (the vertical AF state) may only be *metastable* for these parameter values. The original surface uniform AF state ($\phi_1 = 0$, $\phi_2 = \pi$) may be the global energy minimizer and if the system was perturbed it would relax into the unprimed AF state. Priming would then be necessary to achieve thresholdless switching.

DISCUSSION

We have presented a theoretical model of switching in an AFLC material confined between surfaces which induce polar surface anchoring. We have demonstrated how two thresholdless switching modes may be primed from AF ground states. The first, a twisted smectic thresholdless mode, is stabilized below the smectic C - smectic C_A phase transition by the presence of a quadrupolar ordering term in the free energy. The second, a vertical AF thresholdless mode, is obtained from the uniform AF state by two priming steps which involve breaking of the anchoring constraints at each of the cell surfaces.

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References

[1] P. Rudquist, J. P. F. Lagerwall, M. Buivydas, F. Gouda, S. T. Lagerwall, N. A. Clark, J. E. Maclennan, R. Shao, D. A. Coleman, S. Bardon, T. Bellini, D. R. Link, G. Natale,

M. A. Glaser, D. M. Walba, M.D. Wand and X.H. Chen, *J. Mat. Chem.*, **9**, 1257, (1999).

[2] B. Park, M. Kakata, S. Seomun, Y. Takanashi, K. Ishikawa and H. Takezoe, *Phys. Rev. E*, **59**, R3815, (1999).

[3] I. Dozov, P. Martinot-Lagarde and G. Durand, *J. de Phys. Lett.* **43**, 365 (1982).

[4] G. Durand, F. Simoni, *Appl. Phys. Lett.* **44**, 504 (1982).

[5] G. D. Boyd, J. Cheng and P. D. T. Ngo, *Appl. Phys. Lett.* **36**, 556 (1980).

[6] J. Fünfschilling and M. Schadt, *J. Appl. Phys.* **66**, 3877 (1989).

[7] N. A. Clark and S. T. Lagerwall, *Ferroelectrics* **59**, 25 (1984).

[8] J. S. Patel, *Appl. Phys. Lett.* **60**, 280 (1992).

[9] S. Inui, N. Iimura, T. Suzuki, H. Iwane, K. Miyachi, Y. Takanishi and A. Fukuda, *J. Mater. Chem.* **6**, 671, (1996).

[10] S. Seomun, Y. Takanishi, K. Ishikawa, H. Takezoe and A. Fukuda, *Jpn. J. Appl. Phys.*, **36**, 3586, (1997).

[11] N. J. Mottram and S. J. Elston, submitted to *Ferroelectrics*, (1999).

[12] M. J. Towler, J. R. Hughes and F. C. Saunders, *Ferroelectrics*, **113**, 453, (1991).