Thresholdless switching induced by polar anchoring in antiferroelectric liquid crystals

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Preliminary communication

Thresholdless switching induced by polar anchoring in antiferroelectric liquid crystals

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We present a novel thresholdless switching mode in an antiferroelectric liquid crystal cell which is stabilized by the presence of polar anchoring at the cell surfaces and the antiferroelectric nature of the material. We also suggest other possible configurations which are induced by strong polar anchoring and possess quite different director structures and optical characteristics.

Thresholdless switching modes have been observed in ferroelectric liquid crystal (FLC) materials, e.g. the deformed helix [1] and twisted FLC devices [2], and in antiferroelectric liquid crystal (AFLC) materials [3]. This type of switching has considerable potential for exploitation in active matrix or thin film transistor displays since it exhibits an analogue grey scale, wide viewing angle, large contrast ratio and high-speed response. In AFLC materials, a thresholdless mode was first observed by Inui *et al.* [3] and explained in terms of a *random smectic* model where the director correlation between adjacent layers was small. Recent experimental observations [4, 5] suggest that a more realistic model for this behaviour is a twisted smectic structure in which the AF ordering of the material is suppressed and the liquid crystal is in fact in the FLC phase.

In this communication we present a theoretical investigation of the effects of polar anchoring at the cell surfaces and find a thresholdless mode in which the bulk of the liquid crystal is in the AF phase [6]. We have also found that there exist *multiple solutions* of the governing equations and present three such co-existing configurations in the zero voltage ground state. These solutions have quite different director configurations and optical characteristics, as well as different free energy values. Whilst the system will prefer the minimum energy state, other states may be accessed dynamically. We leave a full analysis of these multiple states to a later date.

In our model, 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 figure 1). We also assume that the behaviour may be modelled by considering only 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. The free energy of the smectic layers is then taken as the sum of the energy contributions from electrostatic interactions, elastic deformation of the director and the antiferroelectric nature of the liquid crystalline material.

Since the materials which we are attempting to model have a high molecular spontaneous polarization ($|\mathbf{P}_s| \approx 5 \times 10^{-4}$–$10 \times 10^{-4}$ C m^{-2}) we assume that there

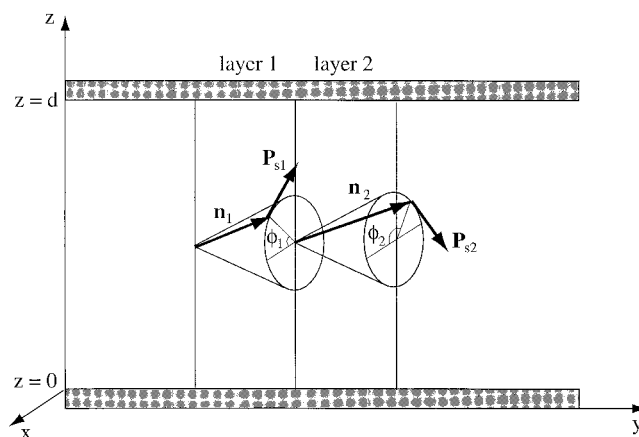Figure 1. Cell configuration: The directors, $\mathbf{n}_1$ and $\mathbf{n}_2$, in layers 1 and 2, respectively, lie on the smectic cone, while the corresponding polarization vectors $\mathbf{P}_{s1}$ and $\mathbf{P}_{s2}$ lie in the xz plane perpendicular to the directors. The layers are in the bookshelf configuration between glass plates at $z = 0$ and $z = d$.

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will be a strong interaction between the surface align-ment layer and the permanent molecular dipole. Thus we assume that the surfaces induce strong polar anchoring such that, at $z = 0$, d, the molecular dipoles are forced to lie parallel to the cell surface normal.

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 $\mathbf{P}_{si} = P_s(-\sin\phi_i, 0, \cos\phi_i)$. The free energy may be written as,

$$
\mathscr{F} = -\frac{\varepsilon_0 V^2}{2d\int_0^1 \frac{1}{\varepsilon_{zz}}\mathrm{d}Z} + \frac{V\int_0^1 \frac{P_z}{\varepsilon_{zz}}\mathrm{d}Z}{\int_0^1 \frac{1}{\varepsilon_{zz}}\mathrm{d}Z}
$$

$$
-\frac{d\left(\int_0^1 \frac{P_z}{\varepsilon_{zz}}\mathrm{d}Z\right)^2}{2\varepsilon_0 \int_0^1 \frac{1}{\varepsilon_{zz}}\mathrm{d}Z} + \frac{d}{2\varepsilon_0}\int_0^1 \frac{P_z^2}{\varepsilon_{zz}}\mathrm{d}Z
$$

$$
+\frac{K\sin^2\theta}{2d}\int_0^1\left[\left(\frac{\mathrm{d}\phi_1}{\mathrm{d}Z}\right)^2 + \left(\frac{\mathrm{d}\phi_2}{\mathrm{d}Z}\right)^2\right]\mathrm{d}Z
$$

$$
+\gamma d\int_0^1 \cos(\phi_1 - \phi_2)\,\mathrm{d}Z \tag{1}
$$

where

$$
P_z = P_s(\cos\phi_1 + \cos\phi_2)/2
$$

and

$$
\varepsilon_{zz} = \varepsilon_\perp + \Delta\varepsilon\sin^2\theta(\sin^2\phi_1 + \sin^2\phi_2)/2
$$

are the average spontaneous polarization in the z direction and the average zz component of the dielectric tensor. In equation (1), the z coordinate has been non-dimensionalized with the cell gap width d so that $Z = z/d$, V is the voltage applied across the cell, ε_0 is the permittivity of free space, K is the Frank elastic constant and γ is the antiferroelectric ordering parameter.

The first four terms in equation (1) describe the electrostatic energy contributions and are derived by solving Maxwell's equations [7] assuming that the electric properties may be averaged over the two layers. It has previously been shown that the presence of a spon-taneous polarization in the layers causes a polarization self-interaction which tends to minimize gradients in $\mathbf{P}_{si}$. Thus in a smectic C twisted layer the bulk of the material will orient such that P_z is constant. However, since the electric properties have been averaged over two layers

the presence of AF ordering (i.e. $\phi_2 = \pi + \phi_1$) leads to zero net polarization such that $P_z = 0$ which corresponds to a minimum in the electric energy. This will be seen more clearly in the next section.

The minimum energy configuration may be found by solving numerically the Euler–Lagrange equations associated with the free energy (1) together with certain boundary conditions. From the assumption that there exists strong polar anchoring of the director at the surfaces, the boundary conditions are $\phi_i = 2n\pi$ on $Z = 0$ and $\phi_i = (2m+1)\pi$ on $Z = 1$ for any integers n and m. Thus at the lower cell surface the director is tangential to the surface on one side of the cone (i.e. $\phi_i = 0, \pm 2\pi, \ldots$) while at the upper surface the director lies on the surface on the opposite side of the cone (i.e. $\phi_i = \pm\pi, \pm 3\pi, \ldots$).

We now have a full mathematical description of the system. In order to solve this minimization problem, we employ the numerical continuation package AUTO97 [8, 9] which will not only calculate a solution to the Euler–Lagrange equations, but also investigate the behaviour of this solution and the system as certain parameters vary. It is able to detect bifurcation and limit points and thus find multiple, co-existing solutions for a specific set of parameter values.

We now consider the results. If we initially assume the polar anchoring is such that ϕ_1, $\phi_2 = 0$ at $Z = 0$ and $\phi_1 = \pi$, $\phi_2 = -\pi$ at $Z = 1$, then within a single layer the director must rotate from one side of the cone to the other, but this rotation is in opposite directions for adjacent layers. We have found that such a configuration leads to thresholdless switching.

Figure 2(a) shows the azimuthal angle solutions and the change in the component of polarization along the z axis as the voltage is changed for the parameter values $d = 2\times10^{-6}$ m, $K = 10^{-11}$ N, $P_s = 5\times10^{-4}$ C m^{-2}, $\gamma = 5$ N m^{-2}, $\theta = 25°$, $\varepsilon_0 = 8.85\times10^{-12}$ F m^{-1}, $\Delta\varepsilon = -1.5$ and $\varepsilon_\perp = 5.0$ (for large values of the spontaneous polarization P_s and antiferroelectric ordering parameter γ the behaviour of the system is qualitatively the same). For zero volts there exists a boundary region near to the lower cell surface where the director reorients from being on one side of the cone ($\phi_1 = \phi_2 = 0$) to being in an AF state ($\phi_1 = \pi/2, \phi_2 = -\pi/2$). There is a corre-sponding boundary region at the upper surface where the director reorients from being in this AF state ($\phi_1 = \pi/2, \phi_2 = -\pi/2$) to being on the opposite side of the cone ($\phi_1 = \pi, \phi_2 = -\pi$). This configuration in the bulk is stabilized by the AF ordering and the electrostatic energy terms.

As the voltage is increased from zero the bulk orientation continuously transforms to the field aligned state ($\phi_1 = \phi_2 = 0$) so that the spontaneous polarization vectors are now parallel to the field in the z direction.
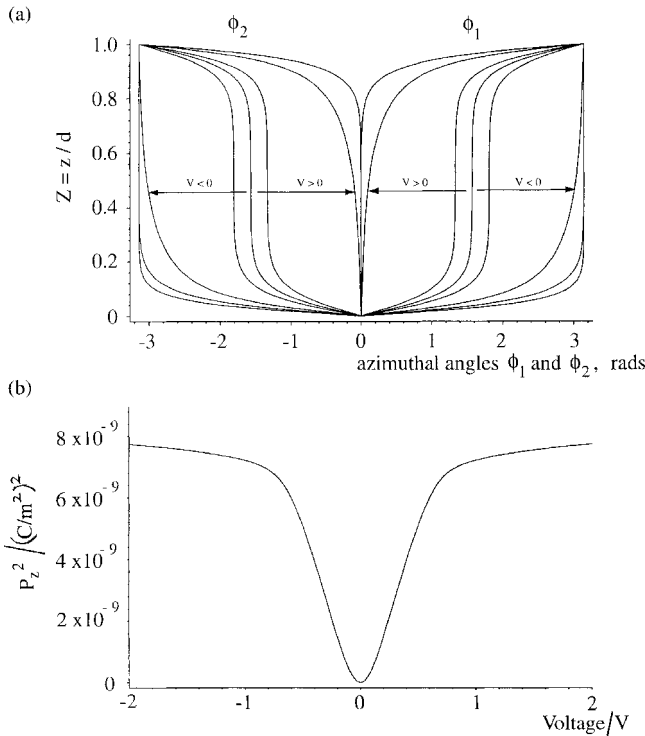
(a)

(b)

Figure 2. Thresholdless switching mode. (*a*) The azimuthal angle configurations $\phi_1(Z)$ and $\phi_2(Z)$. When $V = 0$, the bulk of the cell is in an AF state with $\phi_1 = \pi/2$ and $\phi_2 = -\pi/2$. As the voltage increases or decreases from zero, the directors continuously reorient towards 0 or π F states, respectively. (*b*) The square of the component of the spontaneous polarization in the z direction, P_z^2 versus the applied voltage V showing the thresholdless switching between the AF and F states.

Similarly, as the voltage is decreased from zero, the polarization vectors again align with the field in the $-z$ direction ($\phi_1 = \pi, \phi_2 = -\pi$).

Figure 2(*b*) shows how the vertical component of the net spontaneous polarization squared, P_z^2, varies with voltage. At zero volts, the symmetry of the base state ensures that, when integrated over the cell, the net polarization is zero. As the field changes and the polarization aligns in the z or $-z$ direction, the value of P_z^2 increases and eventually saturates. Figure 2(*b*) clearly shows the thresholdless nature of this switching behaviour.

The degeneracy of the boundary conditions allows for the possibility of other configurations of the director. In figure 3 we show three possible solutions of the governing equations when the boundary conditions are $\phi_1, \phi_2 = 0$ at $Z = 0$ and $\phi_1, \phi_2 = \pi$ at $Z = 1$ without an applied voltage. For these boundary conditions, the director must rotate around the smectic cone from one side on the lower cell surface to the other side on the upper cell surface as before, but now this rotation is in the same direction in adjacent layers.
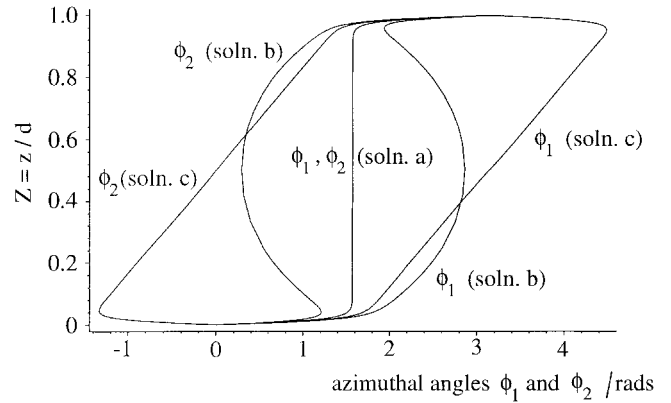

Figure 3. Three co-existing solutions to the Euler–Lagrange equations when there is no applied voltage for parameter values $d = 2 \times 10^{-6}$ m, $K = 10^{-11}$ N, $\mathbf{P}_s = 5 \times 10^{-4}$ C m^{-2}, $\gamma = 5$ N m^{-2}, $\theta = 25°$, $\varepsilon_0 = 8.85 \times 10^{-12}$ F m^{-1}, $\Delta\varepsilon = -1.5$ and $\varepsilon_\perp = 5.0$. In solution (a) the azimuthal angles, ϕ_1 and ϕ_2, in each layer are identical.

The three solutions shown in figure 3 exist at the same parameter values as the $V = 0$ solution in figure 2, but have different free energies. For solution (a) the azimuthal angles in adjacent layers are equal and form a twisted smectic C structure that has been previously studied by Rudquist *et al.* [4] in order to explain the thresholdless behaviour in apparently AFLC materials. In solution (b), the AF ordering energy dominates and leads to a reorientation of the bulk of the cell towards the ($\phi_1 = 0, \phi_2 = \pi$) state. Solution (c) contains a twisted AF state in the bulk of the cell which goes from ($\phi_1 = -\pi/2, \phi_2 = \pi/2$) close to the upper surface to ($\phi_1 = \pi/2, \phi_2 = 3\pi/2$) at the lower surface with boundary reorientation regions. The respective energies of solutions (a), (b) and (c) are -3.723×10^{-4}, -3.799×10^{-4} and -3.843×10^{-4} J m^{-2} (the energy of the $V = 0$ solution of figure 2 was -3.823×10^{-4} J m^{-2}). The magnitude and relative order of these energies will depend on parameters such as the amount of AF ordering γ, the elastic constant K and the magnitude of the spontaneous polarization P_s. However, for the present parameter values, solutions (b) and (c) are stable (solution (c) is the globally minimum energy and solution (b) is metastable), whilst solution (a) is unstable.

Since we are assuming that the director at the boundaries is strongly anchored (with infinite anchoring energy), the solutions in figure 3 are topologically different from the solution in figure 2. Therefore, even though the $V = 0$ solution in figure 2 is of higher energy than solution (c), it cannot be perturbed into the lower energy state. This would of course be possible if we allowed for weak anchoring at the surfaces.

As well as different director structures, these three solutions will have quite different optical characteristics. For instance, solution (a) is essentially a tilted uniaxial

state (with some small boundary regions) which will be optically uniaxial, while solutions (b) and (c) are optically biaxial in the bulk of the cell.

It is worth noting that such multiple solutions could explain the 'priming' effect in some AFLC cells [10]. In such cells, the initial $V = 0$ state (i.e. when the cell has been allowed to relax to a statically stable configuration) is thought to be different to the dynamically accessed zero voltage state (i.e. at $V = 0$ during the application of a periodic voltage which switches the cell between the AF and F states). Thus one of the solutions in figure 3 may be the statically stable state which undergoes hysteretic switching, whilst a different solution may be accessed dynamically and exhibit thresholdless switching.

In summary, we have investigated theoretically a thresholdless switching mode which is induced by polar anchoring at the cell surfaces in a surface stabilized AFLC cell. As a voltage is applied to the cell, the initial AF ordered bulk configuration transforms smoothly into an F state in which the spontaneous polarization vectors align with the electric field. We have also demonstrated that there exist multiple solutions of the governing equations which may account for the 'priming' effect seen in some AFLC cells. The field induced switching (which may be thresholdless or hysteretic) and stability boundaries of these solutions will be discussed in a subsequent paper.

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