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Bistable and monostable polarized states of a liquid-crystalline ferroelectric in an electric field

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A condition for obtaining bistable states in a liquid-crystalline ferroelectric (S_C^*) has been found by computer simulation and analytical estimates; it depends on the value of the applied electric field, the magnitude of the polar contribution to anchoring energy and the material parameters of S_C^* .

1. Introduction

High-speed switching of a ferroelectric smectic C liquid crystal (S_C^*) with a linear electro-optic effect combined with the possibility of obtaining bistability (or optical memory) makes it possible to design a new class of liquid crystals displays, with a high information content; these have been implemented in some cases [1–3]. The creation of bistability conditions has been described in a large number of experimental [4–6] and theoretical [6–9] papers. In the latter the director distribution in the S_C^* was calculated by computer simulation methods. The starting equations in such simulations are the Euler equations for the functional of the free energy for S_C^* [10].

The purpose of this paper is to investigate, using such modelling techniques, how the bistable state in the S_C^* depends on the magnitude of the electric field, the polar contribution to the S_C^* director–substrate anchoring energy, the material parameters of the S_C^* and the initial conditions.

2. Qualitative estimation

Proceeding from the equation of motion [10], certain qualitative assessments of the repolarization process behaviour in thin films of the S_C^* ferroelectric phase, are

$$PE \sin \phi + g\theta^2 \frac{\partial^2 \phi}{\partial y^2} = \gamma\theta \frac{\partial \phi}{\partial t}. \quad (1)$$

Here P is the spontaneous polarization, g is the elastic modulus, γ is the viscosity, θ is the polar angle, assumed to be constant, and $\phi(y)$ is the azimuthal angle for the polarization vector orientation. The boundary conditions can be written as

$$Q \sin \phi_s = g\theta \left(\frac{\partial \phi}{\partial y} \right)_s, \quad (2)$$

where ϕ_s and $(\partial \phi / \partial y)_s$ are values of the azimuthal angle and its derivative at $y = 0$ and $y = d$, d is the film thickness, Q is the effective energy of the polar interaction with the film surfaces. In the absence of the field, E , stationary solutions of equations (1) and (2) are $\phi = 0$ and $\phi = \pi$, provided the anchoring energy, Q , is relatively small, i.e. $Qd \ll g\theta^2$. For the inverse inequality, i.e. a relatively large energy, Q , the stationary

solution takes the form

$$\phi = \frac{\pi g \theta^2}{Qd} + \left(\pi - \frac{2\pi g \theta^2}{Qd} \right) \frac{y}{d}, \quad (3)$$

which is energetically more favourable.

For low surface anchoring energy the external field, E , switches the system from the $\phi = 0$ state into the $\phi = \pi$ state and vice versa. Note that after switching off the field the film must remain in one of these states, as there are no other solutions. Such a situation corresponds to the so-called bistability of the system, having in this case two equivalent states of thermodynamic equilibrium. For large anchoring energy and a not very strong field, E , the initial azimuthal distribution (equation (3)) must not be severely distorted and after the field is switched off the system must return to the initial state, which implies that the system is monostable.

A natural question is whether bistability is possible for strong anchoring of the polarization with the surface if the switching field is sufficiently large and consequently the distortion of the initial structure orientation is also large. We can find the asymptotic behaviour of the solution for $\phi(y, t)$ for the long term effect of the field, E , during time, t , considerably exceeding the characteristic relaxation time τ :

$$\phi(y, t) = \Phi(y) + \psi(y) \exp(-t/\tau). \quad (4)$$

Substitution of equation (4) into equations (1) and (2) gives (accurate to terms of order $\exp(-t/\tau)$) equations for the functions $\Phi(y)$ and $\psi(y)$:

$$PE \sin \Phi + g\theta^2 \frac{d^2 \Phi}{dy^2} = 0, \quad (5a)$$

$$(\tau^{-1} \gamma \theta + PE \cos \Phi) \psi + g\theta^2 \frac{d^2 \psi}{dy^2} = 0, \quad (5b)$$

with the corresponding boundary conditions

$$Q \sin \Phi_s = g\theta^2 \left(\frac{d\Phi}{dy} \right)_s, \quad (6a)$$

$$Q \cos \Phi_s \psi_s = g\theta^2 \left(\frac{d\psi}{dy} \right)_s. \quad (6b)$$

It is clear physically that at $t \gg \tau$ the initial azimuthal distribution (equation (3)) will vary drastically because the polarization must be parallel to the applied field almost throughout the film thickness except for a narrow region near one of its surfaces, where the boundary condition presets the opposite polarization direction. Solution of equations (5a) and (6a) is not difficult and shows that

$$\Phi(0) \approx (2^{1/2} g \theta^2 / Q \xi) \ll 1,$$

where $\xi = (g\theta^2/2PE)^{1/2}$ is the characteristic width of the narrow region near the surface at $y = 0$, $\pi - \Phi(d) \ll 1$.

The function

$$V(y) = -PE \cos \Phi$$

fulfils the role of the potential in the Schrödinger equation (5b) and (6b), the value of $H = (\gamma\theta/\tau)$, the role of the energy and the quantity $M = (2/g\theta^2)$, the role of mass.

The lowest positive eigenvalue of H^* determines the switching time, $\tau^* = (\gamma\theta/H^*)$. For high field values, E , and anchoring energy, Q , the potential $V(y)$ has an almost flat bottom and high walls; this corresponds to the boundary condition $\psi_s \ll 1$. The depth of the narrow potential valley at $0 \leq y \leq \xi$ is of the order of $2PE$. At $\xi \ll d$ the switching time is $\tau^* \approx (\gamma\theta/PE)$.

In fact, the anchoring energy, Q , determines the wall height of the potential trough, V , at $y = 0$ and $y = d$ depending upon the mass-like term, M . In the potential valley near the edge at $y = 0$ this mass must possess sufficiently large kinetic energy $(M\xi^2)^{-1} \approx 2PE$ to overcome the potential barrier and find H^* at an energy level. When the field, E , is sufficiently large, the magnitude of the angle $\Phi(0) \approx (MQ\xi)^{-1}$ approaches π , i.e. the external field overcomes the surface field and the distribution of the azimuthal angle in the film becomes homogeneous ($\Phi = \pi$). After the field is switched off, the system remains in the new state $\phi = \pi$, because the energy, Q , is below the potential barrier $PEf \approx (Mf)^{-1}$, which must be overcome in order to return the system to the initial state. Thus, at $Q < (M\xi)^{-1}$ there occurs a bistability effect. At $Q \gg (M\xi)^{-1}$ the surface anchoring strength is sufficiently large to overcome the potential barrier $PE\xi$ (here the mass M has a rather large impulse ξ^{-1} and proper kinetic energy). In this case the system is monostable, because after the field is switched off it returns to the initial state. The condition

$$Q \approx (M\xi)^{-1} \approx (g\theta^2 PE)^{1/2} \tag{7}$$

is critical for existence of the bistability effect and depends essentially on the anchoring energy, the elastic constant, the tilt angle and the external field.

3. Numerical modelling

Let us rewrite equation (1) as

$$\frac{\partial^2 \phi}{\partial y'^2} + \alpha \sin \phi = \frac{\partial \phi}{\partial t'} \tag{8}$$

where

$$\alpha = \frac{PEd^2}{g\theta^2}, \quad t' = \frac{\gamma\theta d^2}{g\theta^2}, \quad y' = y/d, \quad 0 \leq y' \leq 1$$

with the boundary conditions

$$\frac{\partial \phi}{\partial y'} = \omega_p \sin \phi |_{y'=0,1}, \quad \omega_p = \frac{Qd}{g\theta^2} \tag{9}$$

and the initial condition

$$\phi(y')|_{t'=0} = \pi y'. \tag{10}$$

The problem posed by equations (8)–(10) was solved numerically by the Gears method [11] with a time step $\Delta t' = 0.01$ with specific values of the field energy (α) and the anchoring energy (ω_p). At the initial computation stage the field was switched on and the parameter α (field) had a specified value. Computation continued up to the first stationary solution (S_c^* distorted by the field). The time for obtaining the first stationary solution was fixed, the field was switched off ($\alpha = 0$) and the computations continued until the second stationary solution (S_c^* in the process of relaxation) was found. In figures 1–3 a sequence of solutions for equation (8) for various values of t is presented when the electric field is switched on ($\alpha \neq 0$) and switched off ($\alpha = 0$).

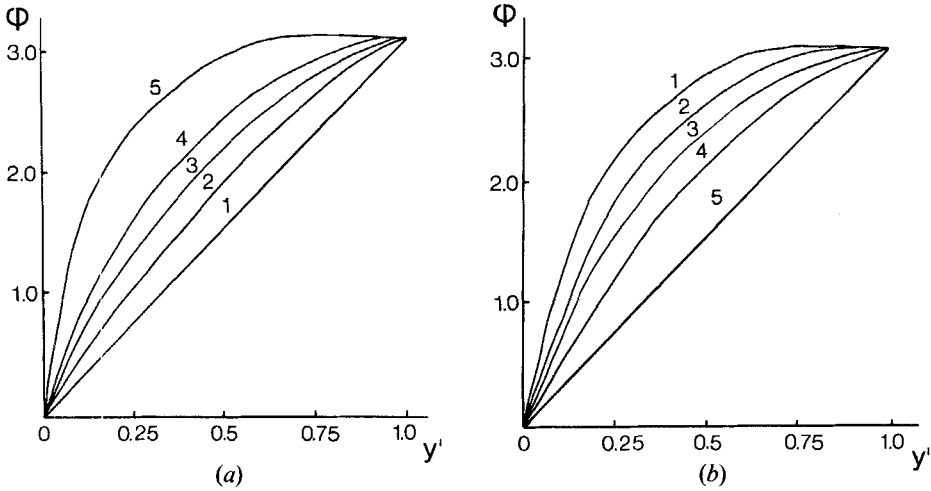


Figure 1. Evolution of the director distribution ($\omega_p = 80$) $\phi(y')|_{t=0} = \pi y'$ for rigid boundary conditions. (a) Distortion in the field $\alpha = 40$ (equation (8)). Curve 1, $t' = 0$; curve 2, $t' = 0.01$; curve 3, $t' = 0.02$; curve 4, $t' = 0.05$; curve 5, $t' = 0.22$. (b) Relaxation process at $\alpha = 0$. Curve 1, $t' = 0$; curve 2, $t' = 0.01$; curve 3, $t' = 0.02$; curve 4, $t' = 0.08$; curve 5, $t' = 0.29$.

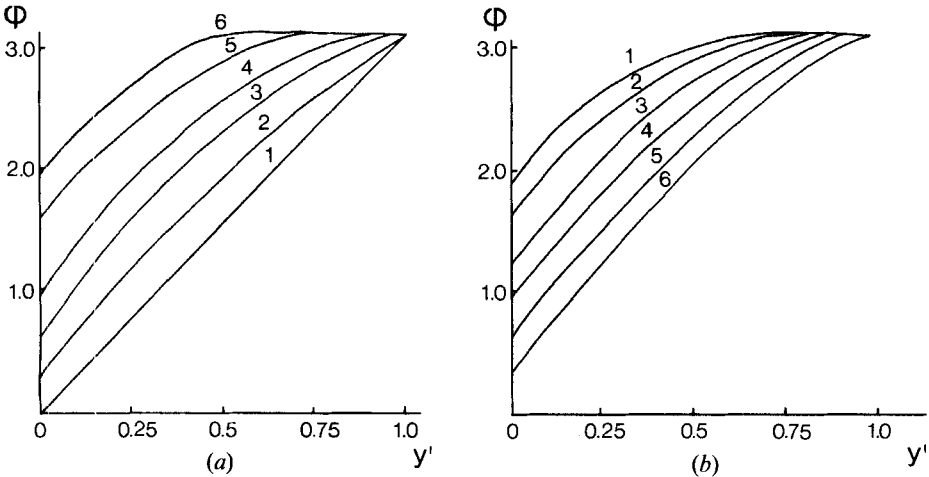


Figure 2. Evolution of the director distribution for a reduction of the anchoring energy ($\omega_p = 8$). (a) Distortion at $\alpha = 40$: 1, $t' = 0$; 2, $t' = 0.01$; 3, $t' = 0.02$; 4, $t' = 0.03$; 5, $t' = 0.08$; 6, $t' = 0.35$. (b) Relaxation at $\alpha = 0$: 1, $t' = 0$; 2, $t' = 0.01$; 3, $t' = 0.02$; 4, $t' = 0.04$; 5, $t' = 0.08$; 6, $t' = 0.39$. It can be seen that the director does not return to the initial state.

For a large anchoring energy and a weak field the director is rigidly fixed at its ends and only in the layer centre is it distorted by the field. When the field is switched off the director returns to the initial state (see figures 1a and 1b). For a low anchoring energy and a strong field the director breaks off and when the relaxation process is over the director in S_C^* does not return to the initial state (see figures 2a and 2b).

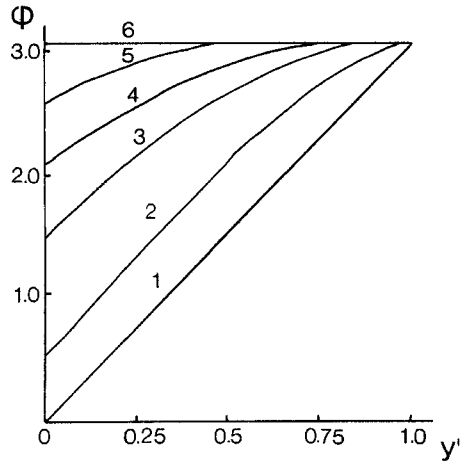


Figure 3. Occurrence of bistability. $\alpha = 100$, $\omega_p = 5.0$. 1, $t' = 0$; 2, $t' = 0.01$; 3, $t' = 0.02$; 4, $t' = 0.03$; 5, $t' = 0.04$; 6, $t' = 0.15$. The distribution described by curve 6, $\phi = \pi$ ($0 \leq y' \leq 1$), does not relax when the field is switched off.

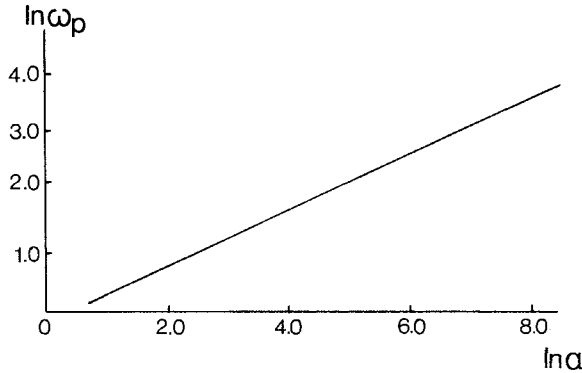


Figure 4. Conditions for obtaining bistable states in S_C^* . The region above the curve corresponds to monostability, under the curve bistability is achieved. Approximate equation for the curve is $\ln \omega_p = \frac{1}{2} \ln \alpha$ or $\omega_p = \alpha^{1/2}$.

At certain values of α and ω_p a bistable state occurs (see figure 3). In figure 3 a stationary solution is demonstrated to be found in the case of bistability. When the field is switched off the director remains in this state for an infinitely long time.

In figure 4 the curve $\ln \omega_p$ versus $\ln \alpha$ is plotted and is a straight line. The space under the curve (lower ω_p values, higher α values) corresponds to realization of bistable states, above the curve (higher ω_p values, lower α values) realization of a bistable state is impossible, i.e. S_C^* is monostable. Numerical calculation of the curve shown in figure 4 is well approximated by the straight line

$$\ln \omega_p = \frac{1}{2} \ln \alpha$$

or

$$\omega_p / \alpha^{1/2} = 1. \tag{11}$$

If we compare equations (7) and (11) considering equation (8), we can see that these conditions are identical, i.e. our analytical estimates are in good agreement with the numerical results.

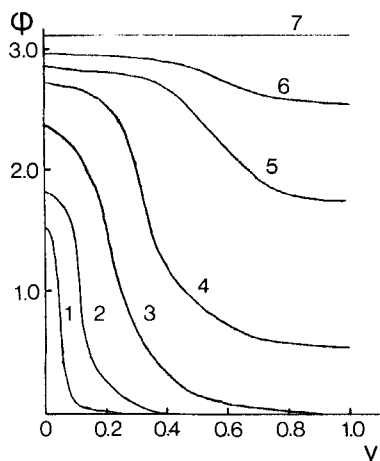


Figure 5. Evolution of solution (12) for the director in a bistable state. $\alpha = 100$, $\omega_p = 0.001$. 1, $t' = 0$; 2, $t' = 0.01$; 3, $t' = 0.03$; 4, $t' = 0.04$; 5, $t' = 0.05$; 6, $t' = 0.06$; 7, $t' = 0.15$.

Figure 5 shows the time evolution of the solution of equation (8) with the initial condition

$$\phi(y')|_{t=0} = \text{arctg}(1/\text{sh } \beta y'), \quad (12)$$

when $\beta = 100$ and $\omega_p = 0.001$. As we can see, in this case bistability (finding a stationary solution $\phi = \tau$) is achieved for the same time as for a uniform twist (equation (10)).

4. Conclusion

Using computer simulation methods and analytical evaluation we have shown that bistabilities (or optical memory) in a surface-stabilized structure of a ferroelectric chiral smectic C can be achieved with various initial director distributions (see equations (10) and (12)) provided the applied electric field E is sufficiently large. That is,

$$E > E_c = Q^2/g\theta^2 P,$$

where Q is the polar contribution of the S_C^* -substrate anchoring energy, $g\theta^2$ is the elastic modulus, P is the polarization of S_C^* . With $E < E_c$ the system is monostable, but with $E \gtrsim E_c$ there is not a complete return to the initial state in the process of relaxation (see figure 2). General consideration of the S_C^* -substrate anchoring energy (taking into account a quadratic contribution and the flexoelectric moment) will be published later.

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