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MODELLING OF SURFACE-STABILIZED FERRIELECTRIC LIQUID CRYSTAL CELLS

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Abstract Two models of ferrielectric liquid crystals are presented. A static model is used if no voltage or a constant voltage is applied to the cell. Six smectic layers would be required to describe the system in full, i.e., to include ferroelectric and antiferroelectric phases as particular cases. A simpler system with three layers has been used for computation restrictions. Switching and hysteresis curves of ferrielectric devices are studied in a second dynamic model in which some static features have been neglected, but viscosity terms have been included.

INTRODUCTION

Surface-stabilized ferro- and antiferroelectric liquid crystal cells have been proposed as an alternative to active-matrix devices for flat panel displays¹. The physical and dynamic behavior of these cells has been studied in a number of works^{2, 3}. If these studies are extended to ferrielectric liquid crystal (FiLC) phases, a general theory for these chiral smectic phases could be developed.

In this work, three-layers static and dynamic FiLC models have been formulated. The least number of layers required for description of an FiLC phase is precisely three. Ferroelectric phases arise as particular cases in these models, while antiferroelectric phases are not included, since an even number of layers is needed for the two-layers periodic structure shown by antiferroelectrics. A six-layers model was formulated, but it resulted unmanageable in terms of computing time. Besides, it is not feasible to induce electrically an antiferroelectric phase from a ferrielectric phase, thus the three-layer restriction is not actually hindering the model capabilities. All three layers share the same shape and the same internal voltage distribution.

MODEL FORMULATION

The system geometry of both models is the same as used in previous work². The static model assumes a chevron structure with no discontinuities at the chevron tip. Five functions are computed: the azimuthal angles of the three layers, $\phi_1(x)$, $\phi_2(x)$ and $\phi_3(x)$, the layer angle $\delta(x)$ and the internal voltage V(x).

The dynamic model employs a simplified geometry with flat layers, a virtual surface at the chevron tip⁴, which becomes discontinuous, and assumes a lineal variation of the internal voltage. The electric contribution includes the dielectric anisotropy and biaxiality. The dynamic model computes only three functions: $\varphi_1(x)$, $\varphi_2(x)$ and $\varphi_3(x)$.

Ferrielectric coupling

Two interactions are considered⁵: one between adjacent layers and another between even or odd layers, i.e., layers having another layer between them. These interactions are characterized by two constants, k_1 and k_2 . Therefore the energy of the *i*th layer is made of four terms corresponding to interactions with layers i-2, i-1, i+1 and i+2:

$$f_{c} = \sum_{i=1}^{3} \left[\frac{k_{1}}{2} (\vec{P}_{i} \cdot \vec{P}_{(i-1) \cdot 3} + \vec{P}_{i} \cdot \vec{P}_{(i+1) \cdot 3}) + \frac{k_{2}}{2} (\vec{P}_{1} \cdot \vec{P}_{(i-1) \cdot 3} + \vec{P}_{i} \cdot \vec{P}_{(i+1) \cdot 3}) \right]$$

$$= (k_{1} + k_{2}) P_{s}^{2} [\cos(\varphi_{1} - \varphi_{3}) + \cos(\varphi_{2} - \varphi_{3}) + \cos(\varphi_{1} - \varphi_{2})]$$
(1)

where P_i are the spontaneous polarizations of each layer and % stands for remainder. The material behavior depends on the values of k_1 and k_2 . If k_1 , $k_2 < 0$, the material is ferroelectric as the molecules of all the layers tend to align parallel to each other. If $k_1 > 0$ and $k_2 < 0$ then the material becomes antiferroelectric, as adjacent layers prefer opposite positions but all even layers are oriented in the same direction. The remaining combinations are ferrielectric.

Taking three layers for modelling implies that short and long range interactions are affecting the same layers. Layers next to ith layer, i.e. (i-1)%3 and (i+1)%3 are the same as non-contiguous layers, i.e., (i-2)%3 and (i+2)%3. This feature ultimately overlaps the effect of k_1 and k_2 . In this model the material behavior only depends

on the sum of k_1 and k_2 : if $k_1 + k_2$ is negative, it is ferroelectric, otherwise it is ferrielectric.

Energy densities and Euler-Lagrange equations

The contributions for elastic, surface and electric energy densities are similar to those employed for ferroelectric¹ and antiferroelectric models², but extended to three layers.

The static model solution requires solving Euler-Lagrange equations of the five functions. A 2nd degree differential equation coupled system is obtained:

$$(C \sec 2\delta \cos \varphi_1 + B \sec 2\varphi_1) \frac{\delta_{\xi}^2}{2} - (k_1 + k_2) P_{\theta}^2 d^2 (\sec (\varphi_1 - \varphi_{(i+1)\lambda_3}) + \sec (\varphi_1 - \varphi_{(i+2)\lambda_3}))$$

$$- B \varphi_{i,\xi\xi} - C \cos^2 \delta \cos \varphi_1 \delta_{\xi\xi} + P_{\theta} d \sec \varphi_1 \cos \delta V_{\xi} = 0$$

$$(2)$$

$$C\cos^{2}\delta\left(\sum_{\ell=1}^{3} \operatorname{sen} \varphi_{\ell} \varphi_{\ell, \ell}^{2} - \sum_{\ell=1}^{3} \cos \varphi_{\ell} \varphi_{\ell, \ell} \right) + \left(C\cos 2\delta \sum_{\ell=1}^{3} \operatorname{sen} \varphi_{\ell} + \frac{3A}{2} \operatorname{sen} 2\delta\right) \delta_{\ell}^{2} + \sum_{\ell=1}^{3} \left(C \operatorname{sen} 2\delta \cos \varphi_{\ell} - B \operatorname{sen} 2\varphi_{\ell}\right) \varphi_{\ell, \ell} \delta_{\ell} + P_{s} d \operatorname{sen} \delta \sum_{\ell=1}^{3} \cos \varphi_{\ell} V_{\ell} + \left(-3 \operatorname{A} \cos^{2}\delta - B \sum_{\ell=1}^{3} \operatorname{sen}^{2}\varphi_{\ell} + C \operatorname{sen} 2\delta \sum_{\ell=1}^{3} \operatorname{sen} \varphi_{\ell}\right) \delta_{\ell\ell} + 6 L d^{2} \operatorname{sen} \delta \frac{\cos \delta_{0} - \cos \delta}{\cos^{2}\delta_{0}} = 0$$

$$-P_{s}d\sum_{i=1}^{3}\sin\varphi_{i}\cos\delta\ \varphi_{i,\xi}-P_{s}d\sum_{i=1}^{3}\cos\varphi_{i}\sin\delta\ \delta_{\xi}+3\,\epsilon_{1}V_{\xi\xi}=0 \tag{4}$$

where i takes the values 1, 2, and 3, $\upsilon = \Delta \varepsilon \sec^2 \theta - \partial \varepsilon$, and $\xi = x/d$ is the x coordinate normalized to the cell thickness, and. The system is solved by relaxation methods.

The Ginzberg-Landau equations of the dynamic model, to be solved by the Crank-Nicholson method, are:

$$\begin{aligned} \phi_{1,\zeta} &= \phi_{1,\xi\xi} - \frac{P_{\theta}dV}{B} \operatorname{sen}\phi_{1} \cos\delta + \frac{K_{f}P_{\theta}^{2}d^{2}}{B} \left[\operatorname{sen}(\phi_{1} - \phi_{(1+1)\eta_{3}}) + \operatorname{sen}(\phi_{1} - \phi_{(1+2)\eta_{3}}) \right] \end{aligned} \\ &+ \frac{1}{2} \left(\operatorname{sen}2\phi_{1} \cos^{2}\delta \, \mathbf{v} - \frac{\Delta \epsilon}{2} \operatorname{sen}2\delta \operatorname{sen}2\theta \cos\phi_{1} \right) \frac{V^{2}}{B} \end{aligned}$$

where $\zeta = t/(\eta d^2/B)$ is a normalized time.

The boundary conditions at the plates are the same as used in previous

models^{2,3}, and the chevron tip is considered a virtual surface⁴, thus giving an internal boundary condition.

RESULTS

As scarce information on ferrielectric materials can be found, the system has been solved using starting values for parameters and constants taken from ferroelectric and antiferroelectric comercial mixtures. The ferrielectric coupling constants have been chosen so that $k_1 + k_2 = 10^9$ N m³/ C².

Ferroelectric materials are bistable. Antiferroelectric materials are monostable if no voltage is applied, while two other states can be stabilized by applying a DC voltage. Ferrielectric materials are bistable with no applied voltage, and show two further states if DC voltage is applied. If a positive voltage is applied, all three layers are UP, while if the applied voltage is negative they are DN; their spontaneous polarization is P_s and -P_s, respectively. Two possibilities are found if

Figure 1. Combinations corresponding to possible system states. Arrows stand for UP and DN.

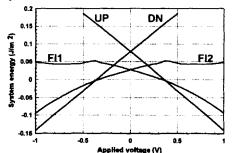


Figure 2. System energy as a function of applied voltage.

no voltage is applied: two layers UP and one layer DN, or two layers DN and one layer UP. The overall polarization of the first case is P_s/3, while -P_s/3 corresponds to the second case. Figure 1 labels every combination of UP and DN layers.

The stability of these states chiefly depends on P, and on the sum of the

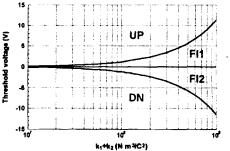


Figure 3. Phase diagram for ferroelectric and ferrielectric states.

coupling constants k, and k₂. Figure 2 show the system energy of every state as a function of the applied voltage. There are three threshold voltages: between DN and FI2, between FI2 and FII, and between FII and UP. The first and third threshold voltages should have the same magnitude but opposite sign; the second should be zero. one Threshold voltages

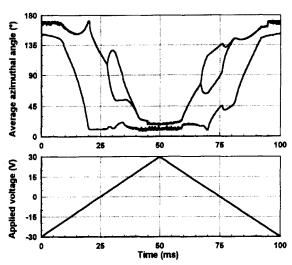


Figure 4. Response of a ferrielectric material to a triangular wave.

different coupling constant values determine a phase diagram (Figure 3) in which the thresholds for the two ferroelectric states increase with the coupling constants, while the FiLC region widens. If the voltage needed for stabilizing the ferroelectric states is known, this graph can be used to get an approximate value of the coupling constant

Transitions between states can be also studied dinamically. Figure 4 shows the results of the dynamic model when a 10 Hz, 30 V triangular wave is applied to the FiLC cell. The lowest voltage at the beginning of the graph stabilizes the DN ferroelectric state. As voltage is approaching 0 V, one of the layers switches (FI2) while the other two layers remain unswitched. Shortly after crossing to positive values, a second layer switches (FI1). Note that the unswitched layer moves opposite to the electric field for a while, as the layer coupling intends to stabilize a ferrielectric configuration. If the voltage is further raised, the third layer switches, and the system reaches the UP ferroelectric state. The second half cycle is identical to the first but in reverse order.

In principle, the existence of four different states in ferrielectric cells suggests

that they could be attractive for video applications. An optical study using the results obtained in the model has been carried out. The ferrielectric states are stable without external applied voltage, while the ferroelectric states require positive (UP state) or negative (DN state) bias voltage during the frame time. If a cell has to be multiplexed, the row signal would have to be symmetric, i.e., DC compensated. If a ferroelectric state is stabilized during the frame time, then the opposite ferroelectric state would have to be also stabilized to compensate the previous bias voltage. Therefore, the row signal would have to be divided into two halfcycles, one for stabilizing the UP or the FI1 state, and another for stabilizing the DN or the FI2 state. On the other hand, the optical range of the cell is determined by the contrast between the UP and the FI1 state, or between the DN and the FI2 states. Both ranges have to be equivalent, so that UP and DN states, as well as F11 and F12 states, should be optically indistiguishable. This can be achieved by placing the first polarizer along the rubbing direction, and crossing the analyzer. However, the contrast of this device is quite low compared to the constrast of a ferroelectric cell, because the ferrielectric states are not dark, as the polarizer does not coincide with the ferrielectric orientations. If tilt angle of the ferrielectric material is high, the ferrielectric states are quite bright and the constrast degrades; if tilt angle is low, the contrast is better, but the brightness decreases. In conclusion, ferrielectric cells do not seem adequate for multiplexed optical video devices.

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