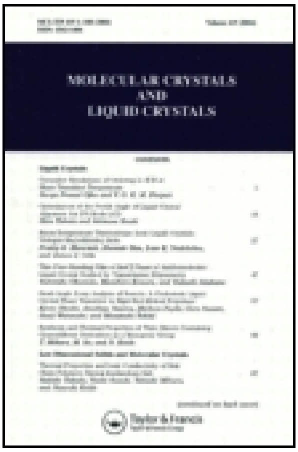

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# Two Dimensional Modelling of Domain Nucleation and Growth in Surface Stabilised Ferroelectric Liquid Crystals

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# TWO DIMENSIONAL MODELLING OF DOMAIN NUCLEATION AND GROWTH IN SURFACE STABILISED FERROELECTRIC LIQUID CRYSTALS

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Abstract In surface stabilised ferroelectric liquid crystal (SSFLC) cells driven by low voltages, typically below 10V, it is observed that domains of the switched state nucleate and grow, merging to fill the cell. A model of domain nucleation in SSFLCs is proposed, which considers a nucleation site as a local absence of the chevron interface torque. The model is implemented in a two-dimensional simulation of the SSFLC SCE-8 in a chevron configuration with C2 alignment. It is shown to behave realistically over the voltage range 2-10V by comparison with experimental results.

## INTRODUCTION

The high switching speed and bistability of ferroelectric liquid crystal (FLC) cells in the surface stabilised geometry, first reported by Clark and Lagerwall[1], allow their use in high density colour screens. Much effort has since been devoted to understanding the switching mechanisms. The simplest model considers the cell to switch homogeneously and uses a balance of electric and viscous torques to predict the cell behaviour. The model has been refined by the inclusion of effects such as layer tilt[2], chevron layer structure[3], ionic transport[3,4], and surface torque[5]. This model works well when the voltage applied to the cell is high, but fails to account for domain growth behaviour observed at lower voltages. Ishibashi[6] has developed an alternative approach based on the Kolmogorov-Avrami (KA) theory[7] of first order phase transitions. In this model domains of switched state nucleate in the unswitched state and grow at a constant rate until the cell is fully switched or the driving force is removed. Ohta et al.[8] have extended this model in one dimension by including a time dependence of the growth rate, which must be known beforehand.

TABLE I SCE-8 parameters.

| Parameter | Symbol | Value |
|---|---|---|
| polarisation | $P$ | $6.3\text{nC/cm}^2$ |
| tilt cone angle | $\theta$ | 19.5 deg |
| layer tilt angle | $\delta$ | 17 deg |
| rotational viscosity | $\gamma$ | 0.16Pa.s |
| dielectric constants | $\epsilon_\perp$ | $4\epsilon_0$ |
|  | $\epsilon_\parallel$ | $5.5\epsilon_0$ |
| dielectric anisotropy | $\Delta\epsilon$ | $-1.5\epsilon_0$ |
| bulk elastic constant | $K$ | 4pN |

In previous work[9] we presented a two-dimensional numerical simulation of a tilted layer SSFLC cell in which the nucleation of domains is assumed at $t = 0$, and in which the number of domains is determined by the magnitude of the voltage pulse applied. In this paper we present a nucleation model for a chevron layer SSFLC cell which predicts the transient creation and growth of a domain.

## THEORY

The cell is modelled as a $2\mu$m layer of SCE8, with parameters listed in Table I, between $0.1\mu$m thick alignment layers (relative permittivity $\epsilon_{AL} = 10\epsilon_0$) with a low surface pretilt. This leads to a perfect C2 alignment at the surface, *i.e.*, the smectic cone 'rests' on the surface such that only one director orientation is stable, as shown in Figure 1(a). A chevron kink is assumed in the mid-plane of the cell.

The general equation governing the rotation of the molecular director $\phi(x, y)$, where $x$ and $y$ are defined in Figure 1(b), is[2]

$$\gamma \sin^2\theta \frac{d\phi}{dt} - K\,\nabla^2\phi$$
$$+PE\cos\delta\sin\phi - \epsilon_0\Delta\epsilon E^2\sin^2\theta\cos^2\delta\cos\phi(\sin\phi - \sin\phi_0) = 0. \tag{1}$$

The four terms correspond to the viscous, elastic, permanent electric, and induced electric torques respectively. $E(x, y)$ is the electric field in the $x$ direction, $\phi_0$ is the angle such that a molecule lies in the $(y, z)$ plane parallel to the surfaces, and $K$ is an average Frank elastic constant. All other parameters are as Table I. The chevron kink can be considered as an interface[10] between the top and bottom of the cell; there is a torque $T$ at this interface which is approximated by

$$T = -\frac{B}{\Delta y}\cos\phi(\sin\phi - \sin\phi_0) \tag{2}$$

where $B$ is an elastic constant and $\Delta y$ is the finite difference spacing. This equation is an adaptation of the Rapini-Papoular torque in nematics[11] $-(K/2L)\sin 2\theta_S$, modified to account for the layer tilt. The surface alignment is approximated by considering

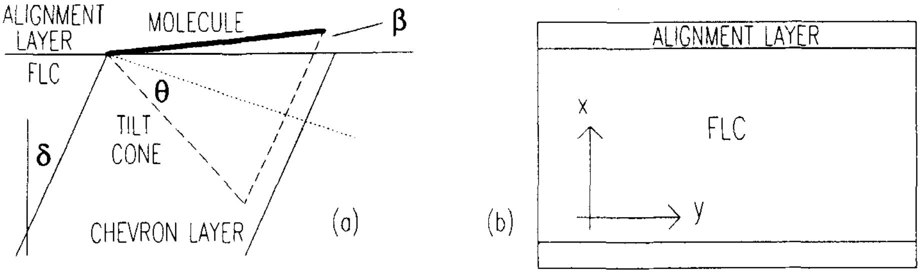

FIGURE 1 (a) Perfect C2 alignment with surface pretilt $\beta$. (b) The plane of the numerical simulation. $y$ is parallel to the alignment layers and $x$ is perpendicular to them.

the alignment layers as another layer of the liquid crystal with fixed orientation and the same elastic constant $K$.

Poisson's equation across the pixel can be written:

$$\epsilon E + P \cos\delta \cos\phi = q(y) \tag{3}$$

where $q(y)$ is the local charge per unit area on the plates of the pixel ($\int q(y)dy = Q$, the total charge on the pixel), and (for all y) $\int E(x)dx = V$, the voltage across the pixel. The integral across the pixel is extended into the alignment layers to take into account any voltage drop across these layers.

Equations (1)-(3) are solved by finite differences in two dimensions, with the solution plane perpendicular to the alignment layers as shown in Figure 1(b). A step by step technique is employed to find the transient behaviour. First the electric field $E(x,y)$ is found using (3) and then the step change $\Delta\phi(x,y)$ is calculated using (1) and (2). This is added to $\phi(x,y)$, the time is advanced and the process repeats. The initial conditions are that at $t = 0$ all elements $\phi(x,y) = \phi_0$.

According to experiments by GEC, in a test cell containing ZLI4655 the threshold between domain switching and homogeneous switching is approximately 10V. To reproduce this in the simulation, the elastic constant $B$ at the chevron interface is adjusted until at 10V, without introducing the nucleation described later, the chevron elements together overcome the barrier presented by the interface torque (2). The value obtained with the above parameters was $B = 0.0036$N/m.

It has previously been observed that for moderate applied voltages domains tend to nucleate at the same points in the cell from pulse to pulse. Consistent with such observations a nucleation centre is introduced by locally reducing the chevron interface torque. This is achieved by setting $B$ in equation (2) to zero (for simplicity) at several adjacent points. In the simulations presented below the width of the site is $d/2$.

We accept that this simple method of introducing a nucleation centre has no physical justification. However in this paper our main interest lies not in the

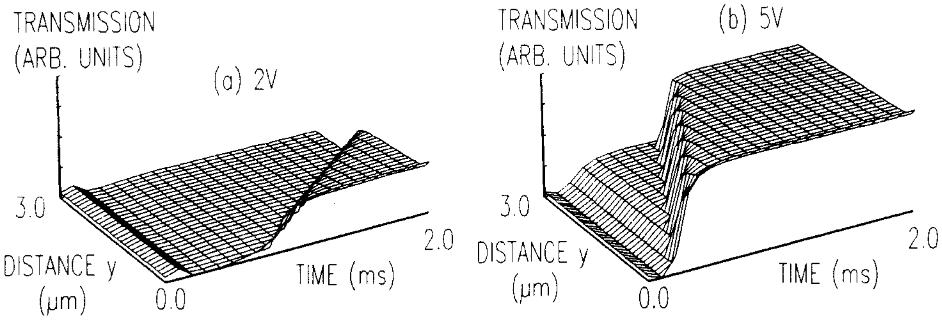

FIGURE 2 Calculated transmission (height) using a 4 × 4 matrix technique as a function of time and distance in the $y$ direction. The nucleation centre is at $y = 0$. The applied voltages were (a) 2V, (b) 5V.

microscopic physical behaviour but in the dynamic consequences of the presence of a nucleation site, and for these purposes the simple method does remarkably well.

Director orientation is recorded throughout the simulation, and optical transmission of 600nm light is then calculated for each point in the pixel at each timestep using the 4 × 4 scattering matrix technique due to Berreman[12].

## DISCUSSION

Simulations of domain nucleation and growth over a range of voltage below 10V (above 10V the liquid crystal reorients homogeneously) were performed. Domain nucleation and growth were not observed in the simulations below 2V.

The transmission as a function of time and distance $y$ is plotted in Figure 2, for 2V and 5V applied voltage. The nucleation site is at distance zero in the figure; its transmission increases more rapidly than that of the bulk of the cell. Only when the bulk has reached an almost constant transmission does the domain wall begin to move away from the nucleation site.

The mechanism for nucleation and growth of the domain is clear: at the start of the simulation the bulk director is unswitched and elastic torque hinders chevron switching; when the bulk moves towards the switched state, elastic interaction contributes to chevron switching. However the total torque is insufficient unless neighbouring chevron elements have already begun switching. Hence for a non-nucleation point, first the director orientation enters a non switched stressed state; as the domain wall crosses the point the region of the chevron switches; and finally the director orientation is forced into a switched stressed state[13].

Notice that the domain wall starts to move significantly after application of the voltage. The time between application of the voltage and domain growth we will call the nucleation time $t_n$. This can be found by extrapolating the position

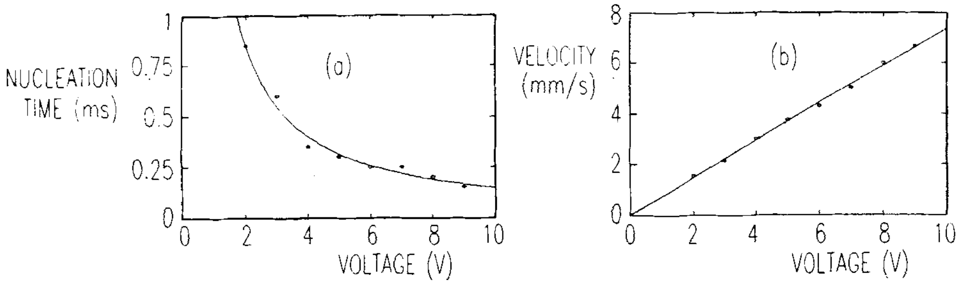

FIGURE 3 (a) Nucleation time $t_n$ as defined in the text, from simulations with varying applied voltage. (b) Simulated domain wall velocity as a function of applied voltage, showing the linear relationship previously observed.

of the centre of the domain wall back in time to the edge of the nucleation site. Nucleation time versus applied voltage is shown in Figure 3(a), fitting the function $t_n \propto V^{-1.1}$ for voltages $V \geq 2\text{V}$. As expected $t_n$ is low for high voltages; it increases rapidly as the voltage decreases, until below 2V it cannot be measured because there is no domain wall movement. (At 1V the simulation was run for much longer than the extrapolated nucleation time, $t_n \sim 1.8\text{ms}$, until there was no further director movement.)

In all the simulations the domain wall quickly achieved a constant velocity after the time $t_n$. This domain wall velocity as a function of applied voltage is shown in Figure 3(b). It can be well described by a linear function $v \propto V$ as observed by Ishibashi[6].

Domain growth is observed at much lower voltages than those for which we have been able to reproduce growth here. This we ascribe to the simplicity of the model of the chevron interface. Despite this, the simulations give useful results over a wide range of voltage around the operating point for a cell in which domain nucleation and growth is the switching mechanism.

## CONCLUSIONS

A domain nucleation model has been proposed and studied in simulations of constant voltage addressing of an FLC cell. Over a useful voltage range the model shows good agreement with experimental data. In particular, for pulses below 10V the model predicts that the material is driven into a stressed state over a time of the order of 0.1–1ms, depending on the applied voltage, prior to the start of domain switching. This is consistent with the observation that at low switching voltages the FLC director reorients into a quasi-static stressed state before the formation of domains and subsequent switching takes place[13].

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