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SIMULATION OF SWITCHING IN ANTIFERROELECTRIC LIQUID CRYSTALS

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Abstract We are simulating the dynamic response of surface stabilised antiferroelectric liquid crystal displays, based on a one-dimensional approach. This leads to more detailed modelling than before[1]. The evolution of director profiles and the resulting optical transmission under applied voltages are studied. The different switching modes between the alternating state and the two uniform states, observed in antiferroelectric test cells, can be understood fairly well. The model incorporates a chevron geometry. The different terms in the bulk energy function can be rationally interpreted. The alignment layers are modelled by a polar and a non-polar surface energy term. The influence of parameters, such as the antiferroelectric coupling parameter, the polar and non-polar anchoring strength, the elastic constant etc. are discussed.

INTRODUCTION

Since the discovery of the antiferroelectric liquid crystalline phase, researchers are spending much effort on the complete understanding of the phase behaviour. This insight has led to a full colour matrix AFLCD prototype, demonstrated at the FLC conference by Nippondensu in 1993[2]. In previous papers[1,3], we presented an analytical model that can explain most of the observed phenomena, including the double hysteresis. Using a uniform bookshelf model, it was possible to study the stable states and the switching behaviour. In our previous model, we assumed no variation of the molecular orientation from bottom till top alignment layer. In this article, we will extend the model to a one-dimensional approach. In other words, elastic forces are now taken into account : the molecular orientation changes throughout the AFLC layer. This allows us to study the evolution of the director profiles. Unlike other models[4], our model incorporates a chevron geometry, polar and non-polar surface anchoring and the influence of the polarisation electric field.

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Although a number of microdomains are often observed during switching in AFLC's[5,6], we do not take into account these effects, i.e. the pixels are assumed to switch homogeneously. This approach can explain most of the observed phenomena.

FREE ENERGY

The antiferroelectric liquid crystal is considered to be a combination of two SmC^* sublattices, coupled by the so-called antiferroelectric interaction. The angles ϕ_1 and ϕ_2 define the position of the liquid crystal molecules on the smectic cone in the even numbered layers and in the odd numbered layers respectively. The definition of the angles is indicated in fig. 1. The position of the molecules on the smectic cone is governed by a minimum energy principle. The total free energy of the liquid crystal can be written as the sum of a bulk energy and a surface energy term.

$$F = \int_V f_{bulk} dv + \int_S f_{surface} ds$$

We are using a one dimensional approach, which means that the angles ϕ_1 and ϕ_2, and thus the bulk energy density, only depend on the coordinate perpendicular to the glass plates of the liquid crystal cell.

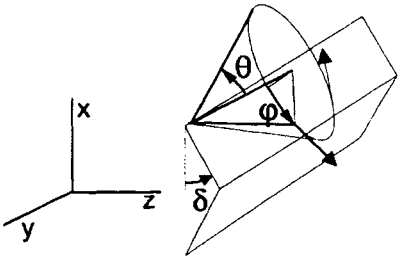

FIGURE 1 Definition of the angles ϕ, θ and δ.

The dynamics of the system can be studied by solving the Euler-Lagrange equations :

$$\frac{\partial f_{bulk}}{\partial \phi_i} - \frac{d}{dx}\left(\frac{\partial f}{\partial \phi_{i,x}}\right) = -\eta \frac{\partial \phi_i}{\partial t}$$

$$\left.\frac{\partial f_{surface}}{\partial \phi_i}\right|_{top} = -\left.\frac{\partial f_{bulk}}{\partial \phi_{i,x}}\right|_{top}$$

$$\left.\frac{\partial f_{surface}}{\partial \phi_i}\right|_{bottom} = \left.\frac{\partial f_{bulk}}{\partial \phi_{i,x}}\right|_{bottom},$$

with i=1,2. η is the rotational viscosity of the liquid crystal material.

For simulations with the chevron geometry, the upper and the lower part of the structure are treated separately, and the chevron interface is considered as an additional surface. At the interface with the alignment layers, $f_{surface}$ is replaced by $f_{alignment\ layer}$; at the chevron interface it is replaced by $f_{chevron\ int erface}$.

The bulk free energy density is the sum of three separate contributions : the elastic energy, the electric energy and the antiferroelectric coupling between the two SmC* sublattices.

$$f_{bulk} = f_{elast} + f_{elect} + f_{AF}$$

For the elastic energy, a simple Oseen -Frank expression is used :

$$f_{elast} = \alpha\left[\left(\frac{\partial \phi_1}{\partial x}\right)^2 + \left(\frac{\partial \phi_2}{\partial x}\right)^2\right].$$

The value of the elastic constant is of the order of 10^{-12} N - 10^{-11} N [6,7].

In the constant voltage mode (passive matrix addressing), the electric part of the bulk free energy can be written as [9]:

$$f_{elect} = -\frac{1}{2}\bar{E}.\varepsilon_0\bar{\bar{\varepsilon}}.\bar{E} - \bar{E}.\bar{P}$$

$\bar{E}$ is the electric field and $\bar{P}$ is the average polarisation : $\bar{P} = \frac{\bar{P}_1 + \bar{P}_2}{2}$; $\bar{P}_1$ and $\bar{P}_2$ are the polarisations in the even and in the odd layers respectively. The spontaneous polarisation of the CS-4001 mixture from Chisso Corp. is 79.8nC/cm^2.

In the constant charge mode (active matrix addressing) another expression has to be used:

$$f_{elect} = +\frac{1}{2}\bar{E}.\varepsilon_0\bar{\bar{\varepsilon}}.\bar{E}$$

The antiferroelectric coupling term is defined as :

$$f_{AF} = A\cos(\phi_1 - \phi_2),$$

where A is of the order of a few 10^3 J/m^3.[6,8]

The interaction of the liquid crystal with the alignment layers is written as the sum of a non-polar and a polar surface anchoring contribution :

$$f_{\text{alignment layer}} = -\gamma_1\left[\cos^2(\Omega_1 - \theta_p) + \cos^2(\Omega_2 - \theta_p)\right] - \gamma_2\left[\vec{P}_1.\vec{s} + \vec{P}_2.\vec{s}\right].$$

In this expression, Ω_i is the angle between the director at the surface and the glass plates, θ_p is the direction of the preferred orientation at the surface and $\vec{s}$ is the outward normal of the surface. γ_1 and γ_2 indicate the strength of the non-polar and the polar surface energy respectively. The value of the surface anchoring constants is of the order of 10^{-4} J/m^2. [6]

The interaction at the chevron interface is described by a surface energy term, similar to the interaction between the alignment layers and the liquid crystal. This surface energy describes the trend of the directors at both sides of the chevron interface to align parallel to each other. We used the following expression[12] :

$$f_{\text{chevron interface}} = -\gamma_3 \cos\chi,$$

with χ the angle between the directors just above and just below the chevron interface. The Euler-Lagrange equations were solved with a computer program, using an implicit difference method. The number of slabs in the x-direction is 50. The optical transmission was calculated by the 2x2 Jones method for normal incidence of the light. For each slab, we averaged the molecular orientation over two consecutive smectic layers. With this averaged molecular distribution, the corresponding Jones matrix was calculated. Simulations were carried out in the bookshelf geometry and in the chevron geometry.

RESULTS

Bookshelf geometry

Figure 2, 3 and 4 show the evolution of the director profiles for the three common switching modes in AFLCD's. In figure 2, the liquid crystal switches from the alternating state to one of the two uniform states. This happens when a DC voltage

higher than a threshold is applied. The smectic layers with the polarisation originally opposite to the applied electric field switch to the other side of the smectic cone (fig.2 right). The smectic layers with the polarisation in the direction of the electric field deviate a little from their initial state ($\phi = 0$) during the switching process (fig.2. left).

The liquid crystal parameters that we used for the simulations were : elastic constant α =4.0x10^{-12} N, rotational viscosity η =100 mPa.s, spontaneous polarisation P=100 nC/cm^2, antiferroelectric interaction A=1500 Pa, non-polar surface anchoring constant γ_1=2.4x10^{-4} N/m, polar surface anchoring constant γ_2=0, surface pretilt θ_p=0°, half smectic cone angle θ=45°, smectic layer tilt angle δ=0, dielectric constants $\varepsilon_1 = \varepsilon_2 = \varepsilon_3$=5. The thickness of the cell is 1.6μm.

Figure 3 shows the switching from a uniform state to the alternating state. Initially, both directors deviate from the uniform state with ϕ=0. In one layer, ϕ evolves to 90°, in the other layer to -90°. After that, the director in the first layers returns back to ϕ=0 (fig.3 right), while the other evolves further to ϕ=-180° (fig.3 left).

In figure 4, the liquid crystal switches directly from one of the uniform states to the other uniform state, which is accomplished by applying a DC electric field opposite to the original polarisation. This switching mode is similar to the switching in ferroelectric liquid crystals. Because of the antiferroelectric interaction, the directors in consecutive layers turn round the smectic cone in the opposite sense.

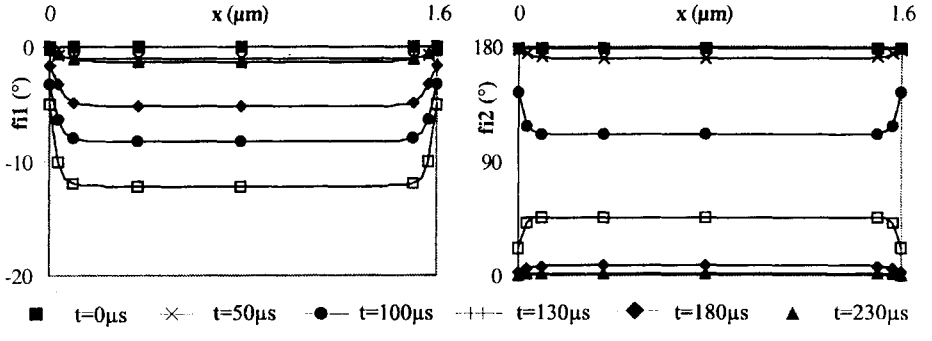

FIGURE 2 Switching from the alternating state to one of the uniform states in the bookshelf geometry.

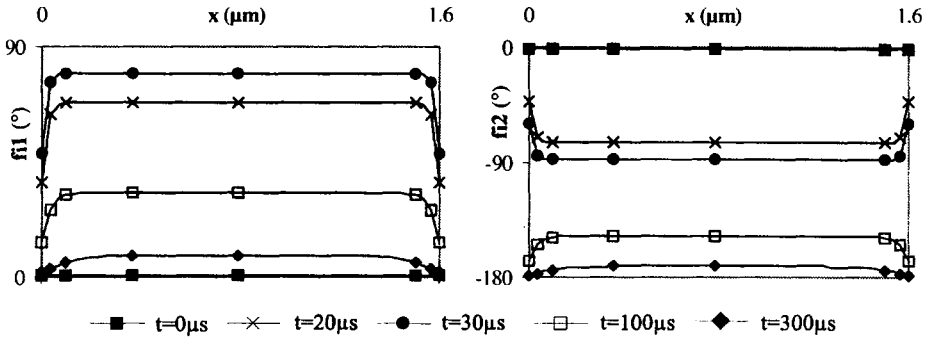

FIGURE 3 Switching from one of the uniform states to the alternating state in the bookshelf geometry.

Figure 5 shows the optical transmission in function of time for the three switching processes. The switching from a uniform state to the alternating state is slower than the opposite process.

Figures 6 and 7 denote the influence of the surface anchoring constants on the director profiles. If the non-polar surface anchoring constant is too large, the liquid crystal does not relax to the alternating state when a zero voltage is applied. Instead, a symmetrical state, with the molecules in both layers at the same side (left side) of the smectic cone appears. This is illustrated in fig. 6. If a large polar surface anchoring constant is assumed (γ_2=2.4x10^{-4} N/m), splayed states appear, see fig.7. Starting from one of the uniform states, the liquid crystal evolves to a splayed state, instead of the alternating state (figure 3). In consecutive layers, the polarisations are anti-parallel in the bulk, but parallel at the surface.

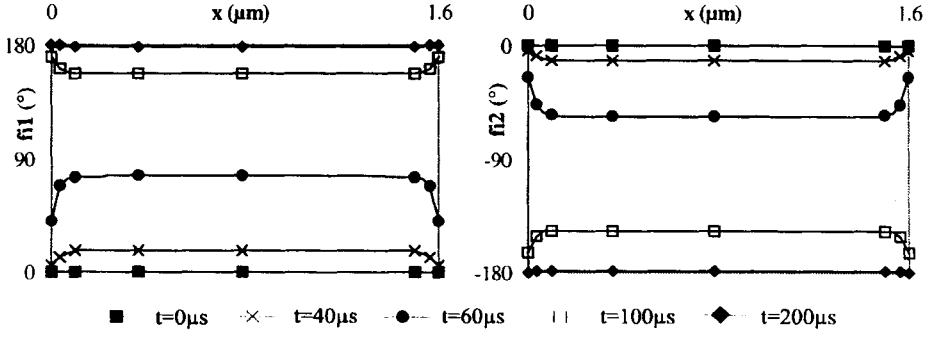

FIGURE 4 Switching between the two uniform states in the bookshelf geometry.

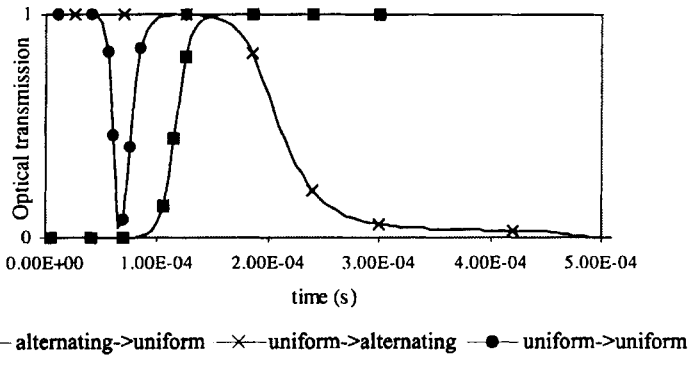

FIGURE 5 Optical transmission for the three switching modes in antiferroelectric LCD's.

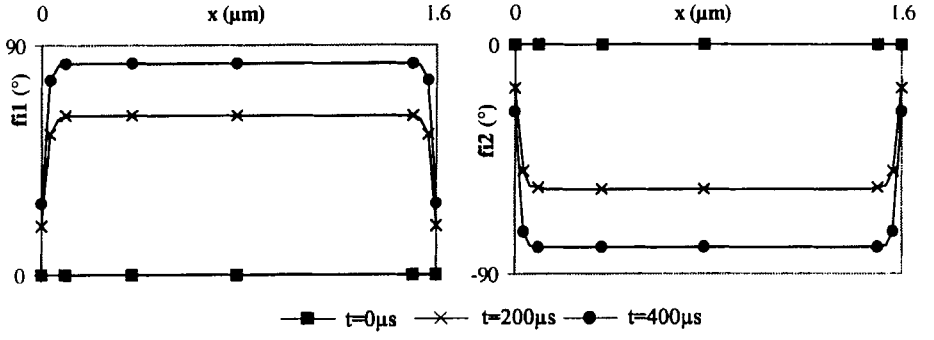

FIGURE 6 If the non-polar surface anchoring constant is too large (γ_1=2.4x10^{-4} N/m), the liquid crystal does not relax to the alternating state.

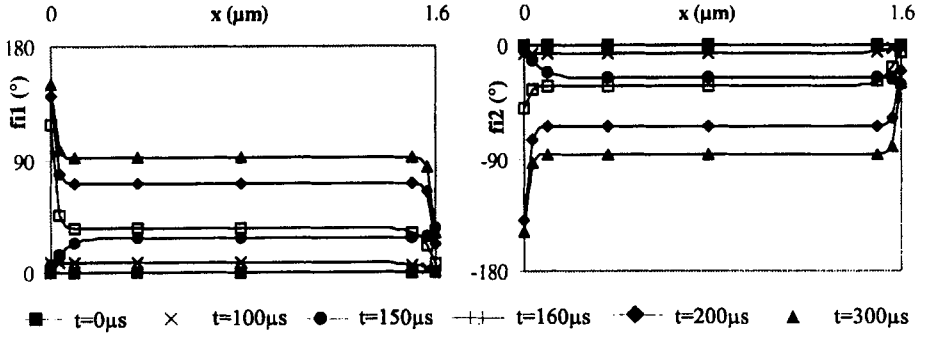

FIGURE 7 If the polar surface anchoring constant is too large (γ_2=2.4x10^{-4} N/m), the liquid crystal relaxes to a twisted state instead of the alternating state.

Chevron geometry

Some authors mention the switching between the bookshelf geometry and the chevron geometry under the influence of electric fields[10]. According to us, this cannot happen without introducing defect structures in the 3rd dimension[11]. We neglected this phenomenon in our one-dimensional model. We used a constant chevron angle of 15°, with the chevron interface in the middle.

Figure 8 shows the evolution of the director profiles while switching from the alternating state to one of the uniform states in the case of a chevron structure. Again, the director in the smectic layer, of which the original polarisation is opposite to the applied electric field, switches to the other side of the smectic cone. The director in the other smectic layer deviates only a little while switching.

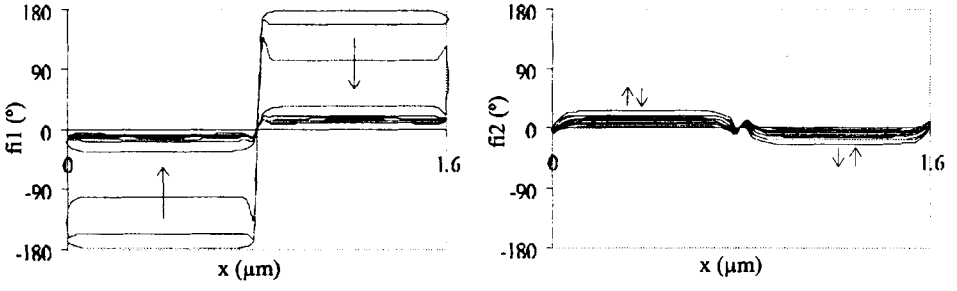

FIGURE 8 Switching from the alternating state to one of the uniform states in the chevron geometry.

Figure 9 illustrates the influence of the antiferroelectric coupling parameter A on the double hysteresis of the transmission. A larger interaction results in a wider hysteresis and an increase of the threshold voltage for the field induced transition from the alternating state to the uniform states. The threshold for switching back also increases. These two results were expected, since a larger value of the antiferroelectric coupling should result in a stabilisation of the alternating state.

The influence of the elastic constant α on the double hysteresis is depicted in figure 10. A larger elastic constant results in a smaller hysteresis.

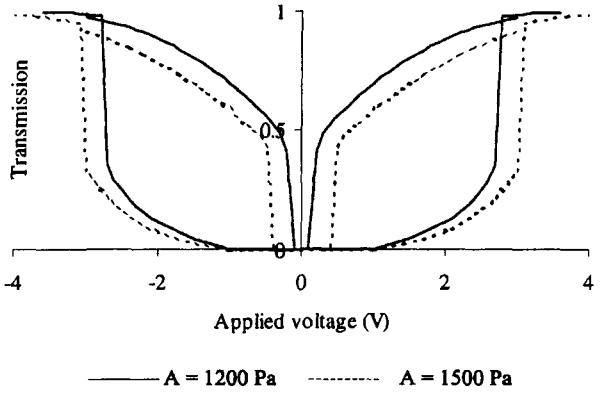

FIGURE 9 Influence of the antiferroelectric coupling parameter on the double hysteresis for the optical transmission.

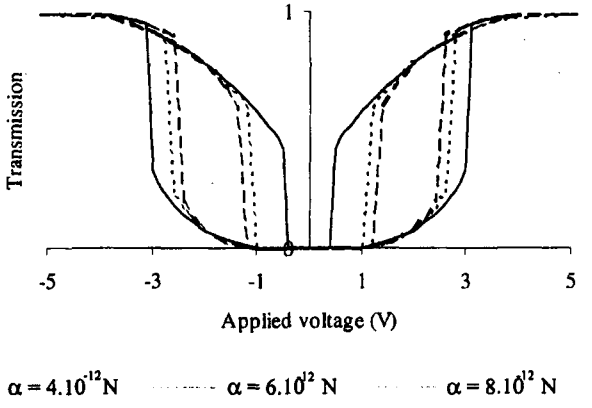

FIGURE 10 Influence of the elastic constant on the double hysteresis for the optical transmission.

CONCLUSION

We studied the switching process in surface stabilised antiferroelectric liquid crystal displays, using a one-dimensional chevron model. The different switching phenomena can be explained and the influence of the different parameters is clear. If the non-polar surface anchoring constant is too large, no normal switching can occur in AFLCD's. If the polar surface anchoring constant is too large, twisted states occur. A larger antiferroelectric coupling constant results in higher threshold voltages, and a larger elastic constant leads to a smaller hysteresis curve.

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