A Novel Approach to Modelling Nematic Liquid Crystal Cells

Christopher J.P Newton, Timothy P. Spiller
Printing & Imaging Technologies Laboratory
HP Laboratories Bristol
HPL-2000-109
24th August, 2000*

computer simulation, liquid crystals, displays

We present a novel lattice modelling approach for the behaviour of nematic liquid crystals in cells. Our model includes elastic deformation energy, finite surface anchoring and applied voltages. These have been implemented and tested in a two-dimensional model. We present results from this model for various analytic test cases and for a real scanning electron micrograph (SEM) surface profile, as employed in experimental work on zenithally bistable nematic devices (ZBN). Finally we discuss, briefly, our extension of the model to three dimensions.

* Internal Accession Date Only
Approved for External Publication

A Novel Approach to Modelling Nematic Liquid Crystal Cells

C. J. P. NEWTON and T.P. SPILLER
Hewlett-Packard Laboratories, Bristol, Filton Road, Stoke Gifford, Bristol BS34 8QZ, U.K.

We present a novel lattice modelling approach for the behaviour of nematic liquid crystals in cells. Our model includes elastic deformation energy, finite surface anchoring and applied voltages. These have been implemented and tested in a two-dimensional model. We present results from this model for various analytic test cases and for a real scanning electron micrograph (SEM) surface profile, as employed in experimental work on zenithally bistable nematic devices (ZBN). Finally we discuss, briefly, our extension of the model to three dimensions.

Keywords Computer simulation; Liquid crystals; Displays

INTRODUCTION

We are interested in displays for electronic paper. These need to have good contrast and to have high resolution, at least 300dpi. Current displays are unable to achieve this and so we are looking at new ways of reaching this goal.

One of the main difficulties when trying to obtain high resolution is the need to refresh the screen regularly. This can be avoided by using a bistable display, pixels are set and remain in that state until they are changed again.

C.J.P. NEWTON and T.P. SPILLER

We are focussing on bistable nematic liquid crystal displays. The liquid crystal (LC) is sandwiched between two micro-structured surfaces and the bistability arises from the boundary conditions that these surfaces, and their surface treatments, put on the LC material[1,2].

We are using modelling to help us to understand what is happening inside the LC cell and also to explore the effect of changing the surface shapes and/or their surface treatments. To do this we need a model, which will find the different possible stable states and which runs fast enough for us to explore the large design space.

LIQUID CRYSTAL MODELLING

We assume that the LC cell is periodic in the *x* and *y*-directions with a period of about 1 micron and is typically between 2 and 10 microns thick (the *z*-direction). The energy of the LC cell is given by

$$U = \int F_{total}\, d\underline{r}.$$

The total energy density is made up of several components, these are:

- The elastic distortion energy density; the sum of splay, twist and bend terms[3,4]

$$F_n = \frac{1}{2}K_{11}(\nabla.\underline{n})^2 + \frac{1}{2}K_{22}(\underline{n}.\nabla\times\underline{n})^2 + \frac{1}{2}K_{33}(\underline{n}\times(\nabla\times\underline{n}))^2.$$

  The *K*s are the elastic constants and $\underline{n}$ is the nematic director. Clearly there is no twist contribution in two dimensions.

- The surface energy density, in the usual Rapini-Papoular[5] form

$$F_s = \frac{1}{2}A_1\left(1-(\underline{n}.\underline{n}_{s1})^2\right)\delta(P_1) + \frac{1}{2}A_2\left(1-(\underline{n}.\underline{n}_{s2})^2\right)\delta(P_2).$$

  Here A_1 and A_2 give the anchoring strengths at the two surfaces, $\underline{n}_{s1}$ and $\underline{n}_{s2}$ are the preferred directions, and $\delta(P_1)$ and $\delta(P_2)$ are delta functions that ensure that these terms only contribute to the total energy at the surfaces (defined by P_1=0 and P_2=0).

- The dielectric energy density[3,4]

$$F_d = -\frac{1}{2}\varepsilon_0\varepsilon_\perp E^2 - \frac{1}{2}\varepsilon_0\varepsilon_a (\underline{n}.\underline{E})^2,$$

  where $\varepsilon_a = \varepsilon_{//} - \varepsilon_\perp$ is the dielectric anisotropy of the LC.
- The flexoelectric energy density. Flexoelectricity is similar to piezoelectricity in solids, deforming the LC generates a polarisation which interacts with any electric field[3,4]. Flexoelectricity is important in switching these devices and so needs to be included. The energy density is

$$F_f = -\left(e_1(\nabla.\underline{n})\underline{n} - e_3\,\underline{n}\times(\nabla\times\underline{n})\right).\underline{E},$$

  where e_1 and e_3 are the flexoelectric coefficients.

Order terms are not included explicitly in our model at this stage of its development. Such terms may be important for a full understanding of these bistable systems. With our present model, some phenomenological allowance for order effects close to surface may be made through choice of the form and strength of the director surface anchoring. It should also be noted that defect-like structures can form in our numerical model, so this type of order effect can occur. (Examples are given later in the paper.)

We need to find the director configuration, which minimises the total energy, and when the electrical terms are included we must also solve Maxwell's equations to ensure that the electric field and director configurations are consistent. In certain simple cases we can solve this problem analytically, but for our bistable cells this is not possible and so we need a numerical method of carrying out this minimisation. The solution of Maxwell's equations can be effected by writing $\underline{E}$ as the gradient of a scalar potential V and finding the potential configuration which minimises the electric energies.

OUR NUMERICAL MODEL

The starting point for our numerical method is to generate an equally spaced lattice covering the LC cell. We need enough cells to get a good representation of the surface profiles, the smallest useful lattice typically has about 16 cells per micron. The results presented here are for 32 cells per micron. The energy density is then discretised and written in terms of the director at a lattice site and its nearest neighbours[6,7]. The total energy is given by

$$U = C \sum_{lattice} (f_n + f_s + f_d + f_f)$$

Where C is the area (in 2D), or volume (in 3D) of a unit cell. The f-terms are the discretised energy densities at a lattice site.

A Monte-Carlo simulation started at a high temperature and correctly annealed will just find the lowest energy state. We want to be able to find other stable energy minima. We know from experiment, that these stable states exist and that they will not necessarily have the same energy. When cooled from the isotropic state cells of this type always cool into the same state, but can be switched into the other state, which is then stable. We have cells, which have retained the same pattern for over a year.

We have a novel method of finding these energy minima. The energy density at a lattice site is used to give an update rule that allows us to calculate the director at a lattice site, which minimises its energy with respect to its neighbours. The lattice sites are chosen at random

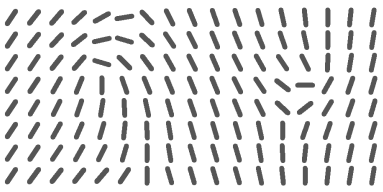

FIGURE 1 An example of the defect structures that arise when the model is started with the directors chosen entirely at random.

and updated immediately so that the new director is used in any subsequent updates. All lattice sites are updated and the procedure started again. Stable configurations are usually achieved after 1,000 iterations, extra iterations then make small adjustments to the configuration and give better results for the total energy. Results presented are for 10,000 iterations (unless stated otherwise).

Starting the system with the directors chosen entirely at 'random' builds in defect like structures which are higher in energy, an example from our 2D model is shown in Figure 1. (In our lattice approach, the defect core size is effectively set by the lattice spacing and defect energies show the expected logarithmic dependence on this cut-off.) These bulk defects can be annealed out, but we avoid this by biasing the initial starting condition (see Figure 2). This also allows us to more easily find different stable energy minima.

The results that we are presenting here are all for equal elastic constants, results for unequal elastic constants will be reported elsewhere [8].

When a voltage is applied across a cell, the electric field is initially uniform. The directors are updated and then the field is updated, followed by the directors again, and then the field, and then … . This procedure is typically repeated five times (10,000 iterations are carried

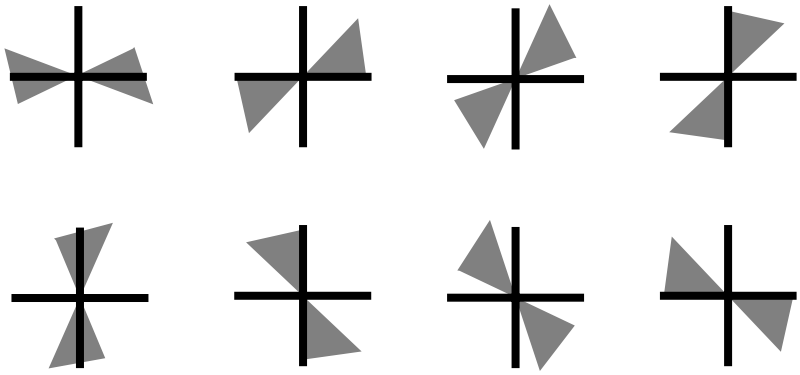

FIGURE 2 Different starting conditions used in the 2D model. Directors are chosen at random from the sectors shown.

out as 5×2,000). The field update is effected through an energy-minimising update rule for the voltage at a lattice site, analogous to that used for the director.

The first results that we show are from some analytical tests for simple cells with planar boundaries where we can obtain the results analytically, or at least by solving an analytic expression. The analytic results are compared with the results from the model and show that the model is working well. These are followed by results for a ZBN cell profile where we are able to obtain director profiles, to show that they are stable with respect to perturbations and to show dielectric switching.

ANALYTICAL TESTS

Weak Anchoring

We test the anchoring terms by using a hybrid cell. The homeotropic anchoring is fixed (∞ anchoring) while the strength of the planar anchoring is given in terms of an extrapolation length

$$l = \frac{K_{11}}{A}$$

For a cell of thickness t the torque balance equation is

$$sin(2\psi) = \frac{2l}{t}\left(\frac{\pi}{2} - \psi\right)$$

Where ψ is the tilt angle at the planar surface. The results from the model are compared with the solution of this equation in Figure 3.

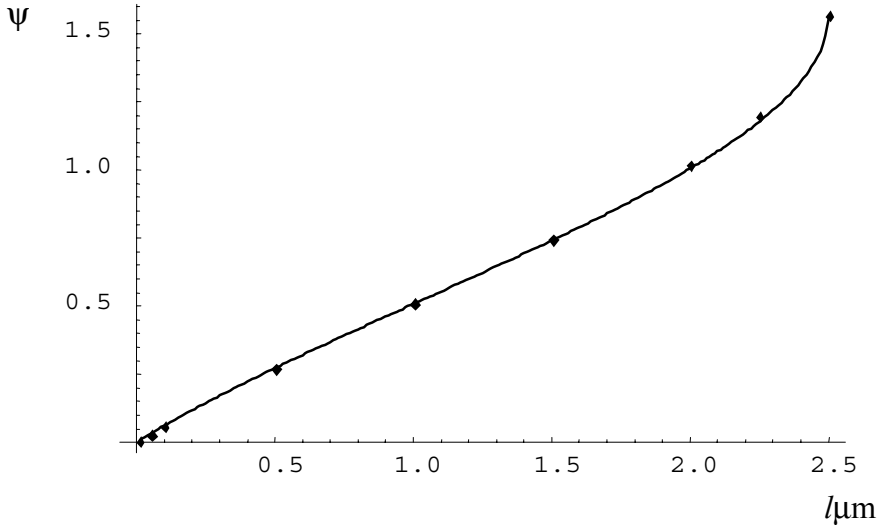

FIGURE 3 Comparison of the analytical and model results for the tilt angle as a function of the extrapolation length, l, for a 2.5μm cell.

Director Update Including Electric Fields

For a planar cell with rigid anchoring and a uniform field applied, the expression for the tilt angle, ϕ, at the centre of the cell as a function of applied voltage is

$$\frac{V}{2}\left(\frac{\varepsilon_a \varepsilon_0}{K_{11}}\right)^{1/2} = \int_0^{\pi/2} d\Lambda \left(\frac{1}{1-\sin^2\phi\sin^2\Lambda}\right)^{1/2}.$$

With a fixed uniform field applied there is a Frederickz threshold, just as in the magnetic case. This threshold is given by

$$V_c = \pi\left(\frac{K_{11}}{\varepsilon_a \varepsilon_0}\right)^{1/2}$$

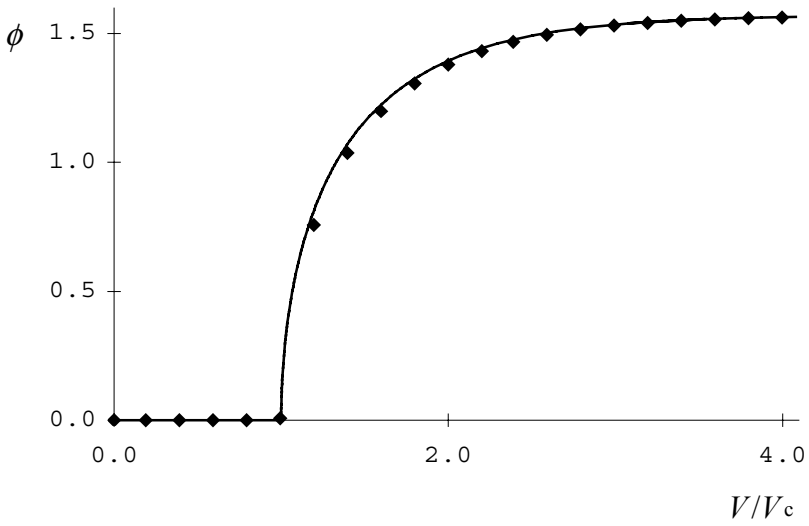

FIGURE 4 Comparison of the analytical and model results for the tilt angle in a planar cell as a function of V/V_c for $Q=0$.

The solution of the equation as a function of V/V_c, together with results from the model is shown in Figure 4. For this test the applied field is uniform, it is fixed at the start and not updated. This test therefore only checks the director update rule. The voltage update has been checked independently against non-trivial analytic solutions to Maxwell's equations

THE ZBN CELL

This type of bistable cell consists of a grating and a planar surface, both treated to be homeotropic. The model was used to obtain director profiles for a cell where the grating used was an image from a SEM of a real cell (see Figure 5). The model was used to obtain stable states for this cell. Three stable states were obtained, these are shown in Figure 6. The v and h-states correspond to those seen experimentally,

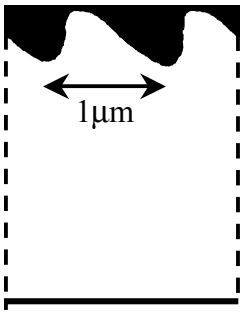

FIGURE 5 A typical ZBN cell. This is periodic in the *x*-direction (horizontal) and invariant in the *y*-direction (normal to the paper). Results shown below are for a 2.5μm thick cell.

while the third higher energy state is not seen (more detailed profiles for this cell, and others, are given in [7,8]). We believe that the high-energy state is an artefact of the 2D constraint of the model. In 3D such a configuration could 'untwist' and indeed results from our 3D model do not show this state. Note that the h-state contains defect structures whereas the v-state does not.

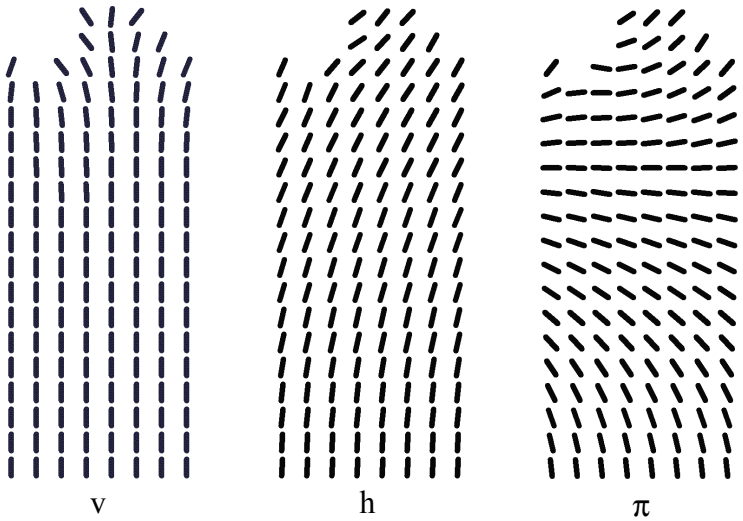

FIGURE 6 ZBN cell profiles obtained from the 2D model.

The profiles shown are for rigid homeotropic anchoring, however these states persist as the anchoring is weakened, eventually disappearing as the anchoring becomes so weak that bulk distortion does not occur.

By applying voltages to the cell we can show dielectric switching from the h to the v state. The final state that we obtain after applying a voltage to the cell, updating and then removing the voltage and updating again is shown in Figure 7. Well above the threshold we have clearly switched into the vertical state. For voltages around the threshold we obtain mixed states, the model cell contains two periods of the grating and these are not identical, one period switches, the other does not.

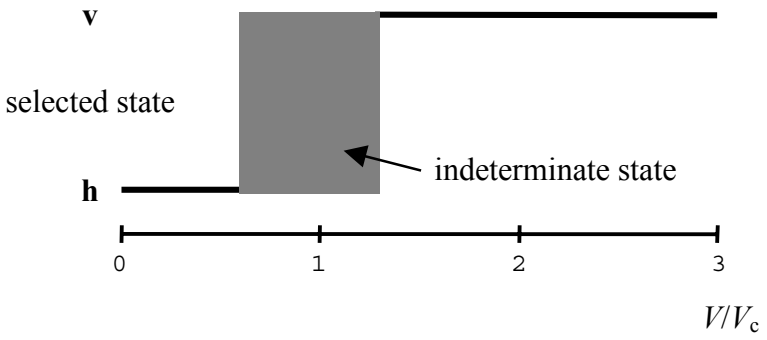

FIGURE 7 'Static' switching from the h to the v state.

Switching from the v to the h state is not so easily demonstrated. Flexo-electricity is important here and we are currently investigating the effect including the flexoelectric terms. Even with these included it is not clear that this type of 'static switching' will work. A dynamical model may well be needed to help us fully understand the switching process.

CONCLUSIONS

We have developed a novel method of finding stable energy states for nematic LC cell that is fast enough to enable us to explore the design space. This model has been demonstrated to work well in 2D although care must be taken when interpreting the results as the restriction to 2D can 'lock-in' states, which would otherwise disappear.

The model is currently being extended to 3D. Early results are encouraging, even with equal elastic constants useful insights can be obtained. We are now implementing other parts of the 3D model and expect to report on these shortly.

Acknowledgements
We thank the authors of reference [2] for providing the experimental grating profile information used for the illustration.

References

[1] G. P. Bryan-Brown, M. J. Towler, M. S. Bancroft and D. G. McDonnell, Proc. IDRC (SID), 209 (1994).
[2] G. P. Bryan-Brown, C.V. Brown, J. C. Jones, E. L. Wood, I. C. Sage, P. Brett and J. C. Rudin, Proc. SID, 37 (1997).
[3] P. G. deGennes and J. Prost, The Physics of Liquid Crystals, Clarendon Press, Oxford (1993).
[4] S. Chandresakar, Liquid Crystals, Cambridge University Press (1992).
[5] A. Rapini and M. Papoular, J. Phys. (Paris) Colloq., **30**, C4-54 (1969).
[6] T. Gruhn and S. Hess, Z. Naturforsch., **51a**, 1 (1996).
[7] C. J. P. Newton and T. P. Spiller , Proc. IDRC (SID), 13 (1997).
[8] C. J. P. Newton and T. P. Spiller in preparation.