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# Molecular Crystals and Liquid Crystals

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## BEHAVIOUR OF A NEMATIC LIQUID CRYSTAL CELL CONTAINING A DIFFRACTION GRATING

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# BEHAVIOUR OF A NEMATIC LIQUID CRYSTAL CELL CONTAINING A DIFFRACTION GRATING

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The director structure of a nematic liquid crystal cell containing a surface relief grating has been modelled using a finite element method. Homeotropic alignment is used, with weak anchoring and the flexoelectric term at the grating surface. The diffraction behaviour of the cell has been modelled using the Finite-Difference Time-Domain (FDTD) method. The liquid crystal's response depends on the sign of the applied electric field and gives different increases in diffraction strength in each case. The changes in the diffraction intensity depend on the surface anchoring and flexoelectric coefficients. Experimental results for cells with a similar structure to those modelled show that the variation of diffraction strength with electric fields of different signs is clearly observable. Results obtained by applying pulses to the cells are presented. These results are compared with the theoretical predictions and are used to estimate the surface anchoring and flexoelectric coefficients.

Keywords: liquid crystal; E7; flexoelectricity

#### INTRODUCTION

If a liquid crystal is composed of molecules with an inherent dipole moment, distortion of the bulk can give rise to a net polarisation. This is known as the flexoelectric effect and was first discussed by Meyer in 1969 [1]. Flexoelectricity is analogous to piezoelectricity (strain induced polarisation) which occurs in certain solids. Recently, interest has been expressed in the flexoelectric effect as it is thought to be a significant factor in the switching mechanism of some bistable device configurations.

Here we discuss an optical method for examining the response of a liquid crystal cell with electric fields of different sign applied to it.

We acknowledge the EPSRC and Hewlett–Packard for a CASE studentship for E. G. Edwards, S. Kitson, C. Newton and J. Rudin at Hewlett-Packard for useful discussions and assistance in production of the chromium complex and L. A. Parry-Jones for useful discussions.

#### **EXPERIMENTAL**

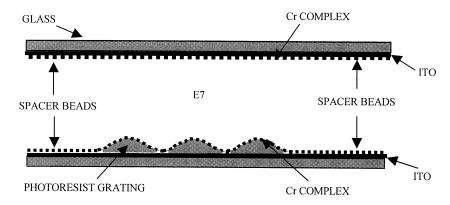
#### The Cell Geometry

A cell was constructed with a surface relief grating on one internal surface. This was written into a photoresist (Shipley S1813) using laser interferometry. The grating had pitch  $1\,\mu m$  and depth  $0.25\text{--}0.3\,\mu m$ . The grating and the flat surface were coated with a chromium complex to give homeotropic alignment. The cell gap was maintained using  $5\,\mu m$  spacers in UV-curing glue. E7 was used as the liquid crystal material. This is shown schematically in Figure 1.

#### The Diffraction Experiment

The response of the liquid crystal when electric fields were applied was investigated by examining the diffraction from the cell. When an electric field is applied to the cell, the liquid crystal realigns. This changes the effective refractive index presented to incident light polarised normal to the grating grooves. The change in effective refractive index alters the index mismatch between the liquid crystal and the grating. Hence the diffraction strength of the grating is changed. For larger electric fields the increase in diffraction strength is larger because the index mismatch increases (for E7  $n_o = 1.521$ ,  $n_e = 1.746$ , for the resist grating n = 1.64). The experimental arrangement to measure the diffraction strength of the cell is shown in Figure 2.

Voltage pulses of 1 ms duration were applied to the cell. Pulses were used to minimise any effects due to ionic migration. The diffraction



**FIGURE 1** Schematic diagram of the cell geometry.

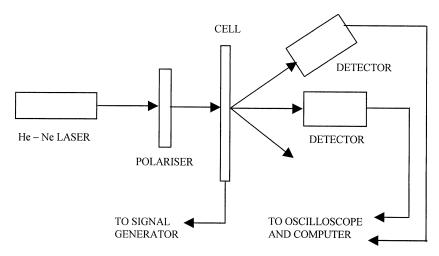


FIGURE 2 Experimental arrangement for the diffraction experiment.

strength was monitored on an oscilloscope and logged onto a computer. Diffraction strength was expressed as the ratio:

 $\eta = 1$ st order strength / 0th order strength

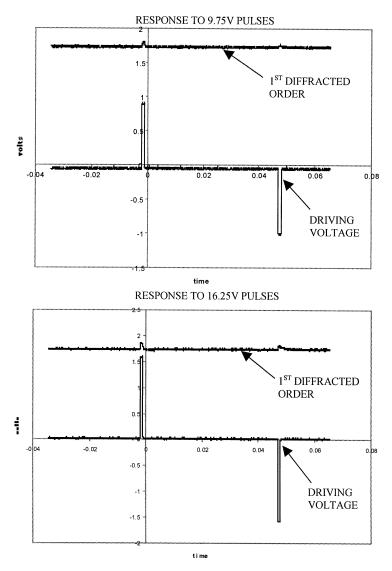
#### Discussion of the Diffraction Behaviour

The response of the liquid crystal to an applied electric field E is due to a combination of dielectric and flexoelectric effects. The dielectric response follows  $E^2$  and so is independent of the sign of E. However the flexoelectric response is linear in E and so depends on the sign of E. The change in diffraction strength showed a dependence on the sign of the applied field. Positive and negative pulses gave different magnitude increases in the diffraction strength, even with high voltages ( $\approx 30$ V). The graphs in Figure 3 show examples of the applied pulse trains and the strength of the first diffracted order.

#### **MODELLING**

#### **Obtaining the Director Profile**

In order to model the optical properties of the cell it was necessary to obtain the director profile. This was achieved using a finite element method [2]. The grating profile was approximated by a sinusoid of pitch  $1\,\mu m$  and depth  $0.3\,\mu m$ . An example director profile is shown in Figure 4.



**FIGURE 3** Examples of the change in diffraction strength when pulses were applied to the cell.

The boundary conditions at the upper surface of the liquid crystal were homeotropic with infinite anchoring. Because most of the distortion takes place in the region close to the grating surface the majority of the device remains homeotropic. It is believed that there is little distortion

#### Approximation to grating aligned cell

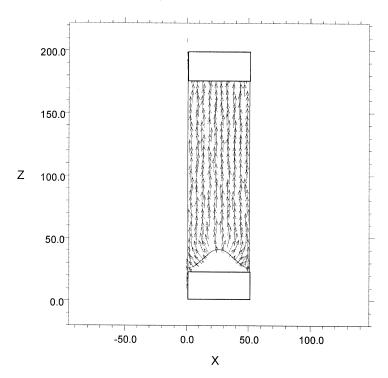


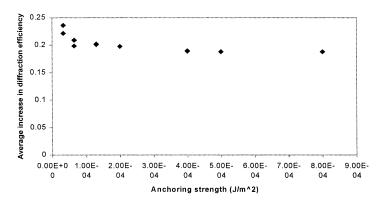
FIGURE 4 An example director profile used in the optical modeling.

at the flat surface and so infinite anchoring was a reasonable approximation. At the liquid crystal/grating surface the boundary conditions were basically homeotropic with weak anchoring. A term representing the flexoelectric effect was also included at this boundary. In the constant electric field approximation flexoelectricity is a surface effect and not included in the expression for the bulk. At the left and right sides periodic boundary conditions were used to eliminate spurious edge effects.

#### **Modelling the Optical Properties**

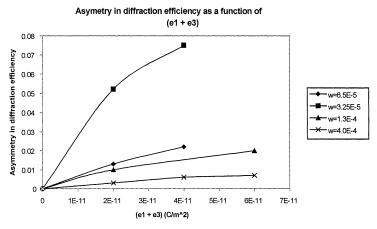
The diffraction behaviour of the cell was modelled using Finite-Difference Time-Domain (FDTD) code developed at Oxford University [3–5]. The diffraction strengths were calculated for cells with different anchoring

## Average increase in diffraction efficiency with 13V pulses as a function of anchoring strength



**FIGURE 5** The change in diffraction efficiency as a function of anchoring strength.

strengths (W) and flexoelectric coefficients ( $e_1+e_3$ ). For strong anchoring (large W) the change in mean diffraction efficiency was largely independent of W. Mean diffraction efficiency was defined by ( $\eta_{positive\ V}+\eta_{negative\ V}$ )/2. It was also seen that the value of W changes the asymmetry in diffraction between positive and negative pulses. The asymmetry in diffraction efficiency was defined by ( $\eta_{positive\ V}-\eta_{negative\ V}$ ). Examples of results from the modelling are shown in Figure 5 and Figure 6.



**FIGURE 6** Asymmetry in diffraction efficiency with  $13\,\mathrm{V}$  pulses applied as a function of  $(e_1 + e_3)$ .

#### **ESTIMATION OF THE FLEXOELECTRIC COEFFICIENTS**

A comparison between the measured mean value of  $\eta$  and that illustrated in Figure 5 shows that the anchoring strength is quite weak, and is near the turning point of figure 5 where the change in diffraction starts to increase. This indicates that the value of W is low, and a value of W=4  $\pm$  1  $\times$  10<sup>-5</sup> Jm<sup>-2</sup> was determined. Measuring the asymmetry in  $\eta$  and comparing with figure 6 shows that for W=4  $\times$  10<sup>-5</sup> Jm<sup>-2</sup> the value of (e<sub>1</sub>+e<sub>3</sub>) is 2  $\times$  10<sup>-11</sup> Cm<sup>-2</sup>. The difficulty in accurately determining the anchoring strength has a consequential effect on the error in (e<sub>1</sub>+e<sub>3</sub>) which is around 25%. Therefore (e<sub>1</sub>+e<sub>3</sub>) = 2  $\pm$  0.5  $\times$  10<sup>-11</sup> Cm<sup>-2</sup>.

#### CONCLUSIONS

The diffraction strength of a liquid crystal cell containing a surface relief grating depends on the sign of the applied field. Comparison between experimental results and modelled data allow estimation of the anchoring strength and flexoelectric coefficients. The value for  $(e_1 + e_3)$  is compatible with other measurements for E7 [6], and the value for the anchoring strength seems reasonable for a homeotropic surface [7,8].

Refinement of the experimental method should allow more accurate determination of these parameters using this approach. The significance of other linear electro-optic effects such as order electricity and surface polarisation need to be considered as these will also influence the response of the cell.

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