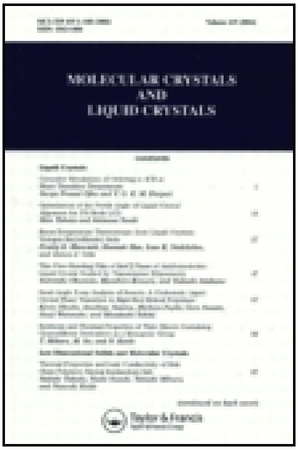

Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

SWITCHING IN LIQUID CRYSTAL FILLED POLYMER STRUCTURES

Stephen Coulston [a] & Garry Lester [a]
[a] Department of Engineering, University of Exeter, North Park Road, Exeter EX4 4QF, United Kingdom

Version of record first published: 07 Jan 2010

Mol. Cryst. Liq. Cryst., Vol. 413, pp. 291/[2427]–303/[2439], 2004

ISSN: 1542-1406 print/1563-5287 online
DOI: 10.1080/15421400490437060

Taylor & Francis
Taylor & Francis Group

SWITCHING IN LIQUID CRYSTAL FILLED POLYMER STRUCTURES

Stephen Coulston and Garry Lester
Department of Engineering, University of Exeter, North Park Road, Exeter EX4 4QF, United Kingdom

Liquid crystal filled polymer structures potentially provide complex switchable optical devices with low driving voltages at low manufacturing costs. The optical properties of such devices are controlled by the shape of the polymer structure and the differences in the refractive index of the polymer and the effective refractive index of the liquid crystal. However, the switching characteristics of the liquid crystal within such devices are strongly dependant on the local geometry of the polymer structure and the alignment layer. Computer simulations using the Landau-de Gennes form of the free energy equation have been used to study this dependence and the interactions involved. These studies have shown that the interaction between the alignment layer on one substrate and the polymer structure induces a small director tilt within the device. As an electric field is applied to the liquid crystal device this induced director tilt affects the switching characteristics of the device and in some cases a strong deformation is observed. Some factors that may affect the development of the observed deformation are presented and discussed here.

Keywords: deformation; grating; Landau-de Gennes; simulation; switching

1. INTRODUCTION

Liquid crystal based devices currently offer a wide range of different switchable optical components, and a number of different technologies are employed in such components. One of these is the Liquid Crystal Filled Polymer Structure (LCFPS) device. The optical properties of these devices depend on both the optical property of the polymer structure as well as that of the liquid crystal. As such these devices offer a number of different switchable optical components that would be economical to manufacture.

Address correspondence to Stephen Coulston, Department of Engineering, University of Exeter, North Park Rd., Exeter EX4 4QF, United Kingdom.

Work has been carried out on a number of simple grating devices [1,2], showing that such devices can be manufactured from readily available materials and that the optical properties of the component can be controlled by the application of an external field. Tests on these simple devices have also shown that their switching characteristics are strongly dependent on the angle between the surfaces of the polymer structure and the preferred direction of orientation of the liquid crystal on the alignment layer. This has significant consequences if the shape of the polymer structure is non-trivial, as different sections of the device will then switch in different ways.

Computer modelling of these devices has been undertaken in order that this dependency can be better understood. A number of unexpected results have been produced, which allow for a better understanding of the observed switching characteristics. It is hoped that these results will lead to new devices where more complicated polymer structures are employed but without unwanted variations in the switching characteristics.

2. BACKGROUND

2.1 Liquid Crystal Filled Polymer Structure Devices

These devices consist of a polymer structure sandwiched between two indium-tin oxide coated glass substrates. The polymer structure is formed onto one of the substrates while the other substrate is treated with an alignment layer, such as nylon 6,6. Figure 1 shows examples of grating structures formed on glass substrates from the photopolymer SU8. When the two substrates have been assembled, the spaces remaining in the polymer structure are filled with a liquid crystal by capillary action.

For clarity in the following discussion, the sections where the polymer has been removed are referred to as the grating channels and the sections where the polymer remains the polymer walls. The direction along the length of the grating channel is the long axis of the channel and the direction perpendicular to this and parallel to the glass surface is the short axis of the channel.

In order to study these devices more closely a number of different grating devices have been manufactured [1,2]. These have allowed various factors to be studied including the period of the grating and the angle between the preferred orientation of the director on the alignment layer and the long axis of the grating. In the grating devices, this angle remained constant along the length of the grating channel and between all grating channels, in a more complex polymer structure this will not necessarily be the case. Thus in order to study the effect of this angle two types of devices have been constructed. The first of these had the preferred direction of the liquid crystal on the alignment layer along the long axis of the grating

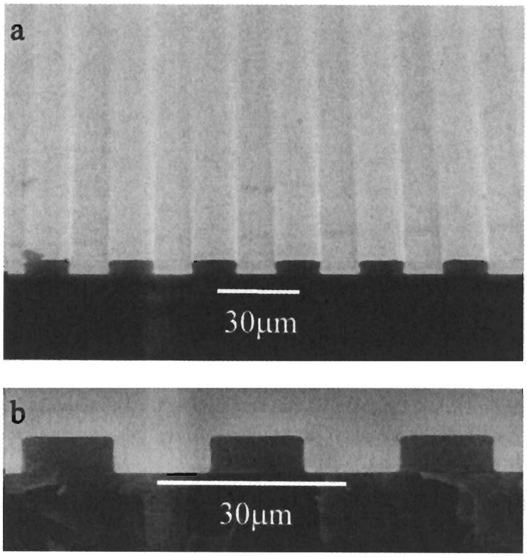

FIGURE 1 Electron microscope picture of a 30 μm periodicity grating.

channel whilst the second had the preferred liquid crystal direction along the short axis of the channel, these devices are referred to as parallel-aligned and perpendicular-aligned devices respectively.

For the devices described above the polymer was chosen such that it had a refractive index between the two refractive indices of the liquid crystal, the photopolymer SU8 and the liquid crystal MLC 6200-100 were used for this reason. This meant that at one particular applied electric field the director would be oriented such that the effective refractive index of the liquid crystal matched that of the polymer. At this point, the device has no overall optical effect, for the grating devices described above this was known as the non-diffracting state. With any other electric field applied to the device, the optical path length through the liquid crystal was different from that through the polymer and this resulted in a diffraction pattern in the far field, which was field dependent.

2.2 Observed Switching Differences in Test Devices

When the parallel-aligned devices were tested, it was found that the switching within the channel was independent of the position along both the short and long axis of the grating channel. As such, these devices provided good contrast between the diffracting and non-diffracting states. However, when perpendicular-aligned devices were tested this was no longer found to be

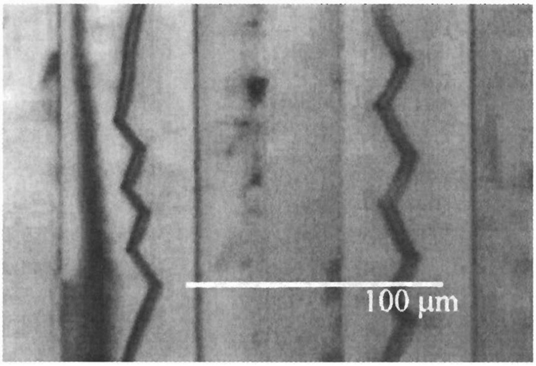

FIGURE 2 A perpendicular-aligned device at 5 V viewed through cross polarizers.

true, instead the switching of the liquid crystal within the grating channel varied along both the short and the long axis of the grating channel. This resulted in the field dependent far field diffraction pattern being complex and there being no non-diffracting state.

When the switching process of the parallel-aligned devices was observed through a polarizing microscope there was a dark line within the grating channel, see Figure 2. This is reminiscent of work carried out by Mori *et al.* [3], in which the grating had been produced by the field from a patterned electrode with the preferred orientation of the liquid crystal on the alignment layer perpendicular to the electrode grating pattern. Mori *et al.* observed that a similar deformation formed in their grating devices and concluded that the deformation seen starts as a low energy defect in the director profile, which then becomes more distinct as an electric field is applied and forms a much higher energy defect. Since the initial deformation has a low energy, it is affected by a number of different local parameters and this accounts for the zigzag nature of the final distinct defect.

3. MODELLING TECHNIQUES

3.1 Introduction to Modelling

Computer modelling has been used to study the observed switching effects seen in the perpendicular-aligned grating devices. Ultimately the model must include the effects of the field within the device due to the applied voltage, the liquid crystal director profile and the optical characteristics of the device. This paper, deals with the computation of the liquid crystal director profile by minimization of the total free energy within the system.

3.2 The Elastic Free Energy Equation

The total energy within the system can be assumed to comprise solely of the elastic free energy within the liquid crystal and the electric potential energy applied to the device [3]. The first of these is governed by the elastic constants of the liquid crystal and the director profile within the device. The second is affected by the voltage applied to the devices, the device geometry and the relative permittivities of all the materials present within the device. The director profile that minimises the total energy within the system is that which is most likely to exist within the device.

Two forms of the elastic free energy equation exist, the Frank-Oseen form [4],

$$f = K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_3(\mathbf{n} \times \nabla \times \mathbf{n})^2 \tag{1}$$

and the Landau-de Gennes form [5]

$$f = \left(\frac{-K_1 + 3K_2 + K_3}{12}\right) P_{jk,l} \cdot P_{jk,l} + \left(\frac{K_1 - K_2}{2}\right) P_{jk,k} \cdot P_{jl,l} + \left(\frac{-K_1 + K_3}{4}\right) P_{ij} \cdot P_{kl,i} \cdot P_{kl,j} \tag{2}$$

where,

$$P_{jk} = n_j n_k - \frac{1}{2}\delta_{jk} \quad j, k, l \in \{x, y, z\} \tag{3}$$

The major difference between the two equations is that the Frank-Oseen equation [1], depends on the vector form of the director, given as

$$\mathbf{n} = \begin{bmatrix} n_x \\ n_y \\ n_z \end{bmatrix} \tag{4}$$

and the Landau-de Gennes equation [2], relies on the tensor form of the director,

$$\mathbf{n} = \begin{bmatrix} n_x^2 & n_x n_y & n_x n_z \\ n_y n_x & n_y^2 & n_y n_z \\ n_z n_x & n_z n_y & n_z^2 \end{bmatrix} \tag{5}$$

The effect of this change in definition is that for the Landau-de Gennes form the following relationship is true, whilst for the Frank-Oseen form it is not.

$$\mathbf{n} = -\mathbf{n} \tag{6}$$

Equation 6 implies that if the angle between the director at two adjacent points is 180° then the directors are equivalent, this is true for most nematic molecules. When this relationships holds the elastic energy calculated between two such points would be zero, however if the relationship doesn't hold then the calculated energy would be very high. Thus the Landau-de Gennes form of the elastic free energy equation remains stable when the director reverses direction between two point whilst the Frank-Oseen equation becomes unstable if the change in the director is greater than 90° between 2 points.

In the system being modelled, the liquid crystal is constrained on all four sides of the channel, on two sides by the polymer walls and on two by the glass substrates. This leads to a high degree of symmetry within the system. Further, in the test devices a distinct deformation was seen to exist within the grating channel, it was therefore expected that the orientation of the director would change by angles greater than 90° within the line of the defect if not between adjacent points. Since it was necessary that the model remain stable at all times it was necessary to implement the Landau-de Gennes form of the free energy equation.

3.3 Special Considerations for Modelling the LCFPS Systems

As mentioned above the elastic free energy within the liquid crystal is dependent on the elastic constants of the liquid crystal and the current director profile. However, the elastic constants for the liquid crystal used in the test devices, MLC 6200-100, are currently unknown so typical values of elastic constants had to be used. It was not possible therefore to complete a quantitative comparison between the model and the test devices, though a qualitative assessment can be made.

The director profile of the liquid crystal within the device was dependent on the alignment of the director at the surfaces of both the glass substrates and the polymer walls. Due to the fabrication method used only one of the glass substrates could be treated with an alignment layer, thus it was only on this surface that the preferred alignment direction is known. When modelling the devices some alignment had to be specified for all of the surfaces, further the model only allowed for alignment in a single direction at each of the surfaces. A preferred direction of alignment had to be assumed at the surfaces of the polymer walls and of the untreated glass substrate. As these surfaces were not treated to give a preferred orientation direction in the real device the assumption of a direction in the model means that the computed director profile can only be an approximation to the actual profile.

A further consideration is that due to computer memory and run time limitations the device must be modelled using a repeated unit cell. The result of this is that the model becomes infinite in two dimensions leading to a uniform grating channel, this makes it impossible to model the zigzag nature of the defect seen in the test devices, Figure 2. Also because of the desire to model the optical characteristics of the device it was necessary that the spacing of the matrix used in the model was 20 nm. This value comes from the requirement in the Transmission Line Matrix (TLM) method [6,7] that the matrix spacing is much less than the wavelength of the light being studied. By using such a fine matrix a large number of points are generated which leads to higher memory and run time requirements, and it is this that limits the overall size of the model possible.

3.4 The Model Geometry

Because of the limitations of the computer resources available the model was restricted to the unit cell shown in Figure 3. This unit cell was a single node thick and repeated boundary conditions were used to generate an infinitely long channel. The distance between each node was set to 20 nm so that the data could be passed directly to the TLM modelling code. The elastic constants used were $k_1 = 14.4*10^{-12}$, $k_2 = 8.0*10^{-12}$and $k_3 = 18.0*10^{-12}$, these were based on the ranges for the ratios of elastic constants suggested by Bahadur *et al.* [8] and the elastic constants used in work by MacGregor [9].

As it was necessary to specify a preferred alignment direction on all surfaces a number of tests were run to find the preferred direction that gave the results closest to observations from test devices. These showed that alignment along the long axis of the grating at both the surface of

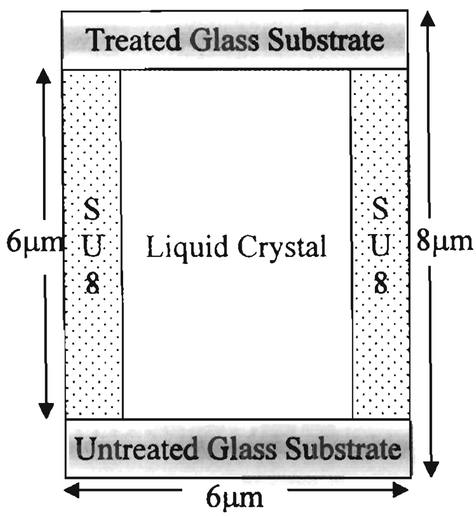

FIGURE 3 Example unit cell.

the polymer walls and the non-aligned glass gave the most realistic results. This alignment may be attributed to the geometric constraints of the device geometry.

4. MODELING RESULTS

4.1 Effect of Surface Pre-tilt and Alignment Direction

In Figures 4 and 6 below the left hand image (a) shows a map of the component of the director along the z-axis (n_z) across the plane of the unit cell. This value varies from +1 to −1 as the director varies from being aligned wholly in the +z direction to being wholly aligned in the −z direction. The contours in these images refer to a change of 0.1 in this value. The right hand image (b) is a graphical representation of the director profile within the device. The light grey areas in these images represent the glass substrates and the dark grey areas represent the polymer walls.

Figures 4 and 6 show the calculated director profile with no applied field when the preferred direction of the alignment layer is along the short axis of the channel in the +y direction. The model in Figure 4 had an alignment layer with no applied pre-tilt whilst the model in Figure 6 had a pre tilt of +6°.

With no pre-tilt applied to the device, as in Figure 4, it was assumed that the orientation of the director would be parallel to the surface of the glass substrate. However, Figure 4a clearly shows that this was not the case and that a director tilt was induced at the point where the polymer surface and

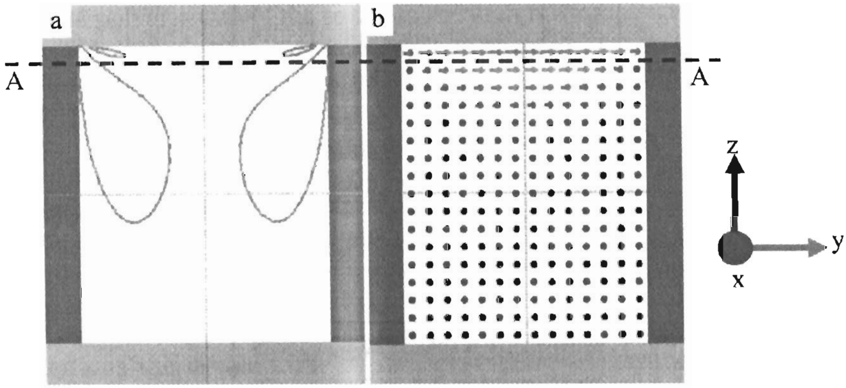

FIGURE 4 Device without pre-tilt, alignment in the positive y direction and no field applied.

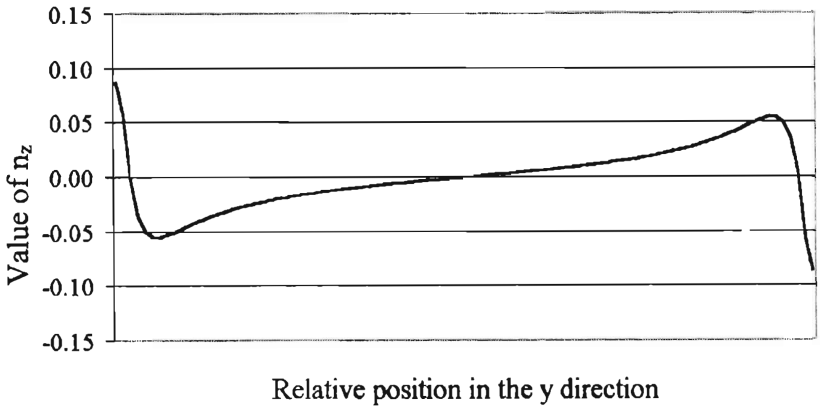

FIGURE 5 Graph of n_z through section A-A in Figure 4.

the alignment layer both interacted with the liquid crystal. As shown in Figure 5 the magnitude of this effect is symmetrical although there is a change in the direction of n_z at the centre of the grating channel.

The effect that this director tilt has on the director profile of the liquid crystal can be seen in Figure 4b where the director appears to bend towards the corners of the grating channel.

Using an applied pre-tilt of $+6^{\circ}$ the director tilt within the device was no longer found to be symmetrical see Figure 6a. The interaction between the

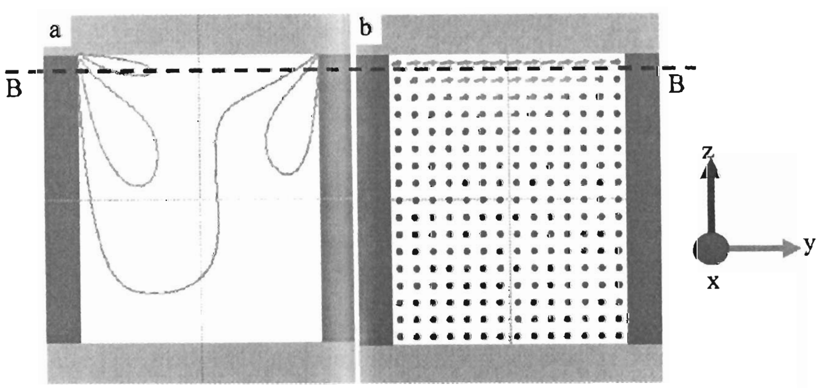

FIGURE 6 Device with pre-tilt, alignment in the positive y direction and no field applied.

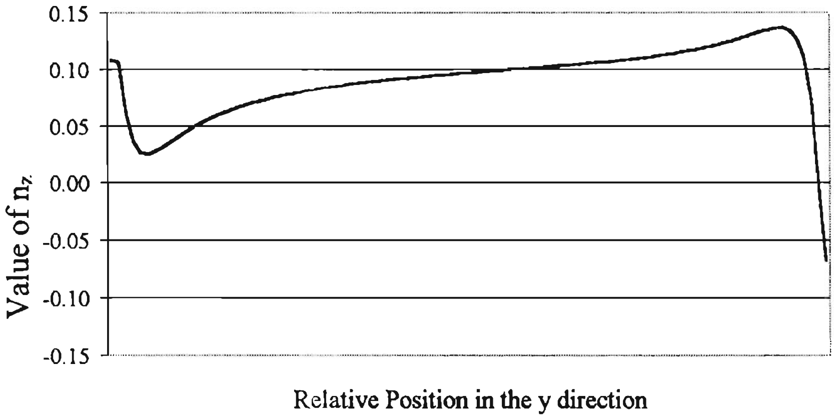

FIGURE 7 Graph of n_z through section B-B in Figure 6.

induced director tilt and the applied pre-tilt has meant that the applied pre-tilt is reinforced on one side of the grating channel and reduced on the other. Figure 6b shows the effect that this has on the director profile within the grating channel.

Figure 7 highlights the non-symmetric nature of the director tilt within the grating channel. In this case a value of 0.1 would represent a pre-tilt angle of 6° and there is considerable variation from this value.

To check that the effects seen in Figures 6 and 7 were due to the alignment direction the same geometry was modelled but with the preferred direction in the $-y$ direction rather than the $+y$ direction. This produced an identical set of results, but with the reinforcement of the pre-tilt on the opposite side of the grating channel as expected.

4.2 Effect of an Applied Field

In the previous section, it was shown that the director profiles for perpendicular-aligned devices are strongly dependent on the preferred direction of the alignment layer and the amount of pre-tilt. In order to show the effect that the director tilts seen in Figures 4 and 6 would have on the switching characteristics of the devices a uniform field was applied to the models. Figures 8 and 9 show the effect of the applied field on the models described in Figures 4 and 6 respectively. The layout and co-ordinate system of Figures 8 and 9 are the same as those of Figures 4 and 6.

Figure 8 shows the effect of applying a field to a device with no applied pre-tilt. In this case the director tilt induced by the combined interaction of

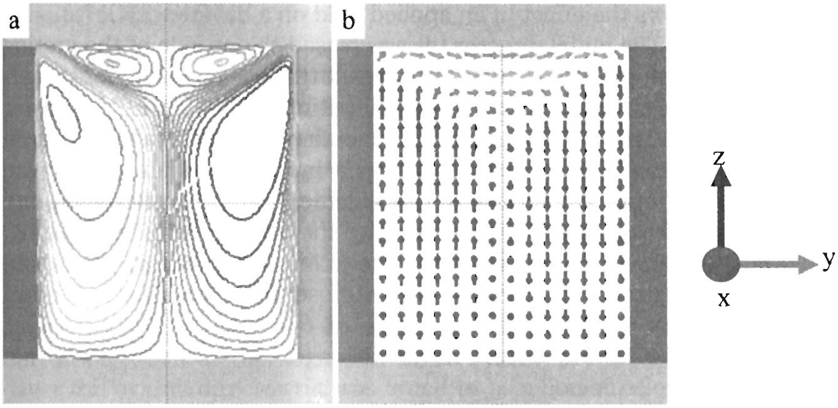

FIGURE 8 Device without pre-tilt, alignment in the positive y direction and with a field applied.

the polymer wall and the alignment layer results in a complex switching pattern. In Figure 4 the director tilt had equal magnitude but opposite direction on opposite sides of the grating channel. With an applied field, the magnitude of the director tilt was increased and the change in the direction of this tilt remained, the result of this was that a distinct and stable deformation formed as shown in Figure 8a and 8b above. This deformation continued throughout the switching process and was strongly reminiscent of the features seen in test devices such as that shown in Figure 2.

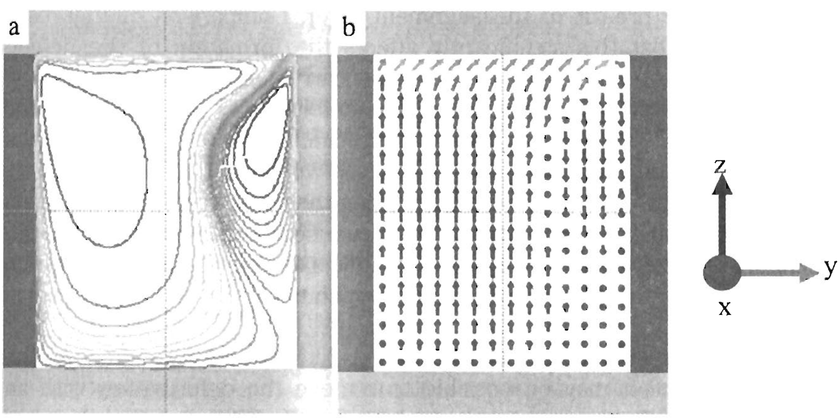

FIGURE 9 Device with pre-tilt, alignment in the positive y direction and with a field applied.

Figure 9 shows the effect of an applied field on a device with an applied pre-tilt of $+6^{\circ}$. The initial director tilt was biased to one side of the grating channel by the applied pre-tilt with the result that the switching of the device was also biased with one side of the grating channel switching faster than the other. This is shown clearly in the director profile at the bottom of Figures 9a and 9b, but can also be seen by close examination of the top of these figures, that is close to the alignment layer. Further, in Figure 7 the director tilt changed direction along the short axis of the grating, however this change in direction was close to one side of the grating channel and from Figure 9 this has been pushed closer to polymer wall as shown in Figure 9a.

5. THE EFFECT OF LOCAL GEOMETRY ON DEVICE SWITCHING

The exact values of the elastic constants for the liquid crystal used in the test devices were unknown, however it is known that typical nematic liquid crystals have a ratio of k_3/k_1 between 0.7 and 1.8 and the ratio of k_3/k_2 between 1.3 and 3.2 [8]. Thus, the values used ($K_1 = 14.4{*}10^{-12}$, $K_2 = 8.0{*}10^{-12}$ and $K_3 = 18.0{*}10^{-12}$) are therefore typical for nematic liquid crystals [8], a more detailed study of the effect of these values on the switching of the LCFPS devices may allow closer comparisons between the model and the test devices. Further, it may be possible to remove or limit the formation of a defect by careful selection of the liquid crystals elastic properties.

A second mechanism for controlling the switching characteristics may be to alter the pre-tilt of the alignment layer. Comparison of Figures 8 and 9 shows that this significantly affects the formation of the defect. Further study of this effect needs to be carried out to investigate the amount of pre-tilt required to move the deformation to the side of the grating channel and whether the pre-tilt can be used to eradicate the deformation. Altering the pre-tilt will have two undesired effects, firstly the change in the optical properties between the state with no applied field and that with an applied field would be reduced with increasing pre-tilt. Secondly it is likely that with higher pre-tilt the device would always switch from one side of the grating channel first which may be undesirable in some cases.

Finally, the profile of the polymer walls is likely to have an effect on the deformation and it may be possible to remove the deformation with an appropriate profile applied to the polymer wall. Changing the shape of the polymer wall is simple within the modelling technique, but may prove more difficult with real devices.

6. CONCLUSIONS

The Landau-de Gennes elastic free energy equation has been successfully applied to the modelling of liquid crystal filled polymer structure devices. This has allowed investigation of the factors that affect the switching of such devices. The current results provide good qualitative agreement with the results seen in real devices.

The modelling has given a fuller understanding of the factors affecting the switching of the test devices. It was shown that with no applied pre-tilt an induced director tilt was present within the device, the shape of which is governed by the combined interactions of the polymer wall and the preferred direction at the alignment layer. With a pre-tilt on the alignment layer the overall director tilt was found to be a combination of the applied pre-tilt and the induced director tilt generating a bias of the director profile to one side of the grating channel.

With a field applied to the model the resulting director profile was found to be strongly dependent on the initial director tilt within the model. Thus, when the model had no applied pre-tilt the result of applying a field was that a deformation forms within the grating channel. This feature compared well with the switching features seen in the test devices.

In the light of the observations made some possible methods for reducing the undesirable switching effects seen have been suggested along with future areas for modelling and device construction.

7. REFERENCES

[1] Strudwick, A. M. & Lester, G. A. (1999). Electrically controlled phase grating for instrumentation applications. *Electron. Lett.*, *16*, 1374–1376.

[2] Lester, G. A. & Strudwick, A. M. (2000). A liquid crystal phase grating for instrumentation applications. *J. Mod. Optic.*, *47*, 1959–1967.

[3] Mori, H., Gartland, E. C., Kelly, J. R., & Bos, P. J. (1999). Multidimensional director modelling using the Q tensor representation in a liquid crystal cell and its application to the π cell with patterned electrodes. *Jpn. J. Appl. Phys.*, *38*, 135–146.

[4] Frank, F. C. (1958). On the theory of liquid crystals. *Discuss. Faraday Soc.*, *25*, 19–28.

[5] Wang-Yang, Li Shu-Hsia, & Chen. (1999). Simulation of normal anchoring nematic droplets under electric fields. *Jpn. J. Appl. Phys.*, *38*, 1482–1487.

[6] Johns, P. B. (1987). Symmetrically condensed node for TLM method. *IEEE T Microw Theory*, *35*, 337–377.

[7] Lester, G. A. (1999). Calculation of optical properties of liquid crystal devices using the transmission line matrix (TLM) method. *Liquid Crystals*, *26*, 1849–1851.

[8] Pohl, L. & Finkenzeller, U. (1990). Physical properties of liquid crystals. In: *Liquid Crystals, Applications and Uses Vol 1*, Bahadur, B., (Ed.), World Scientific: 139–170.

[9] MacGregor, A. R. (1988). Modelling the optical properties of twisted nematic guest-host liquid crystals. *J. Phys. D: Appl. Phys.*, *21*, 1438–1446.