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Quantification of the azimuthal anchoring of a homogeneously aligned nematic liquid crystal using fully-leaky guided modes

B. T. HALLAM*, F. YANG and J. R. SAMBLES

Thin Film Photonics, Department of Physics, University of Exeter, Stocker Road, Exeter EX4 4QL, UK

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A novel optical guided mode technique, the fully-leak y guided mode technique, has been used to investigate the director distortion under the application of an in-plane electric field of a homogeneously aligned conventional cell filled with the nematic liquid crystal E7. The liquid crystal is aligned using polyimide rubbed along the direction of the gold electrode edges. A weak field is applied across a 3 mm gap between the gold electrodes to induce small changes in the twist angle of the director. These distortions are determined by fitting to the angle-dependent reflectivity and transmissivity data and are compared with continuum theory. From careful analysis of the results, both the twist elastic constant, k_{22} , and the azimuthal anchoring strength, W_a , of the system are obtained. At 23.5°C for E7 on rubbed polyimide we find that $k_{22} = (6.50 \pm 0.05) \times 10^{-12}$ N and $W_a = (2.9 \pm 0.2) \times 10^{-5}$ J m⁻².

1. Introduction

As the development and optimization of new liquid crystal electro-optical devices continue, the role of surface alignment remains important. This alignment can be characterized in terms of a zenithal (out of the substrate plane) anchoring energy and an azimuthal (in the substrate plane) anchoring energy. It is these energies that determine to what extent an alignment surfactant will hold a liquid crystal director in a desired orientation and thus how well suited it is to a particular task.

Until recently, research into surface anchoring has concentrated predominantly on zenithal effects. However the desirable viewing angle characteristics obtained through the use of in-plane interdigital electrodes [1] has brought about renewed interest in quantifying azimuthal (in-plane) anchoring.

Broadly speaking, there are two different techniques available for measuring the in-plane anchoring strength W_a . The first makes use of the cell geometry to induce mechanically a twist deformation in the liquid crystal, while the second achieves this via an in-plane field. There have been several reports of work which utilizes the first technique [2–4], with the most common experiment involving the measurement of the displacement of the liquid crystal director away from the easy-axis of alignment at both surfaces of a twisted, homogeneously aligned cell. The analysis of these results relies implicitly on knowing the value of the twist elastic constant k_{22} which is usually obtained via the critical field measurement of a Fréedericksz transition. However Rapini and Papoular [5] have shown that a reduced value of the elastic constant might be obtained if the cell has a finite surface anchoring or if there is a small pre-twist in the cell at equilibrium, which may be difficult to avoid experimentally.

This is not a problem with the external field technique in which an electric or magnetic field is applied in the plane of the homogeneously aligned director to induce a twist distortion. The response of the cell to the applied field is determined by the competition between the applied external torque and the elastic torque of the deformed director. Hence, through careful analysis, the value k_{22} may be determined, as well as W_a . Although some work has been undertaken with the use of in-plane magnetic fields [6-8], there has been very little published on the use of electrical fields [9], possibly due to the increased complexity of the mathematical treatment associated with the anisotropic nature of the material's dielectric polarizability. This complexity is substantially reduced and the resulting data analysis made much simpler if the applied electric fields are kept small. However this has the drawback that the induced director distortions will also be small and hence difficult to quantify by most standard techniques. The sensitivity of optical guided mode techniques to small perturbations of the liquid crystal director profile is well established [10, 11], and for this reason it is ideally suited to this type of study.

^{*}Author for correspondence.

In this work a new guided mode technique, the fullyleaky guided mode technique (FLGM) [12], has been used to examine the twist brought about in a homogeneously aligned conventional liquid crystal cell filled with nematic E7 via the application of an in-plane electric field. By fitting angular dependent reflectivity and transmission data to theory, both k_{22} and W_a have been obtained.

2. Fully-leaky guided mode technique

The FLGM technique combines, for the first time, the sensitivity to the optical tensor profile that is synonymous with guided mode techniques [10, 11] with the ability to examine a commercial cell. This is possible as the cell is no longer constrained by special index glass, as in the half-leaky guided mode technique [10], or by metal layers, as in the method of attenuated total reflection [11]. The geometry of the cell is shown in figure 1: a conventional cell which comprises standard index (n = 1.52) glass is bounded by prisms of an equal refractive index. These prisms are optically matched to the cell by a suitably mixed silicone oil index-matching fluid which allows the cell to be twisted with respect to the prisms. The input prism increases the available in-plane momentum of the incident laser light allowing coupling to a number of leaky modes within the liquid crystal layer. Because both liquid crystal refractive indices are higher than the glass index, these are not true guided modes. These leaky modes lead to broad features in the angle-dependent reflectivity and transmission data. Four sets of transmission data may be collected in addition to the four sets of reflectivity data commonly recorded and can be used to check the resulting model of the director profile. These sets comprise, for reflectivity (R)and transmission (T); p-polarized light incident and p-polarized light recorded (Rpp, Tpp), s-polarized light incident and s-polarized light recorded (R_{ss}, T_{ss}) ; as well



Figure 1. A slice (in the incident plane) through the experimental cell geometry. Alignment of the LC is homogeneous and is close to parallel to the electrode edges. Standard-index glass prisms are optically matched to the cell by a silicone oil matching fluid.

as the polarization conversion signals with p-polarized light incident and s-polarized light recorded (R_{ps} , T_{ps}), and s-polarized light incident and p-polarized light recorded (R_{sp} , T_{sp}). A model of the true director profile will give theoretical reflectivities and transmissivities to fit all eight data sets.

3. Theoretical

The cell geometry comprises a nematic liquid crystal with a twist elastic constant k_{22} and a dielectric anisotropy $\Delta \varepsilon$ homogeneously aligned in the *xy*-plane between two substrates which are separated by a distance d in the z-direction. An electric field \mathbf{E} is applied along the x-axis and the twist angle of the director $\phi(z)$ is measured with respect to the y-axis. It is assumed to be positive for a clockwise rotation along the positive z-direction. The torsional anchoring is assumed to be finite and is generally different on each substrate with strengths W_{a1} and W_{a2} for the top and bottom substrates, respectively. With no applied field, the twist angles at each substrate $(\phi'_{01} \text{ and } - \phi'_{02})$ can be non-zero and do not have to be co-linear with the easy axes of alignment (ϕ_{01} and $-\phi_{02}$). On application of the electric field, the surface twist angles change to ϕ_{d1} and $-\phi_{d2}$. It is important to note at this point that having a small twist in the system with no field applied is actually beneficial experimentally as, in the absence of any chiral dopant, this can break the degenerate nature of the direction of twist induced by the field.

The change in free energy G of a nematic subject to an in-plane electric field may be represented by:

$$G = \int_{-d/2}^{d/2} \left[\frac{k_{22}}{2} \left(\frac{d\phi}{dz} \right)^2 - \frac{\epsilon_0 \Delta \epsilon \mathbf{E}^2}{2} \sin^2 \phi \right] dz + W_{a1}(\phi_{d1} - \phi_{01}) + W_{a2}(\phi_{d2} - \phi_{02})$$
(1)

where the anchoring terms come from the Rapini–Papoular [5] expressions.

The twist deformation is governed by the Euler–Lagrange equation:

$$\frac{d^2\phi}{dz^2} = -\frac{\omega\Delta\varepsilon}{k_{22}}\sin\phi\cos\phi.$$
 (2)

If ϕ is assumed to be small (this is a valid approximation if the fields are kept small) then $\sin(\phi)$ can be linearized and the solution to equation (2) is of the form:

$$z = \xi \sin^{-1} \left(\frac{\phi}{C} \right) + \eta \tag{3}$$

where,

$$\xi = \frac{1}{\mathbf{E}} \left(\frac{k_{22}}{\varepsilon_0 \,\Delta \,\varepsilon} \right)^{1/2}.\tag{4}$$

C is a constant that is dependent on the boundary conditions and η is the value of *z* for which $\phi = 0$, which is also dependent on the boundary conditions.

The twist angles, ϕ_{d1} and $-\phi_{d2}$, are dependent on the torque balance at the two substrates:

$$k_{22} \left(\frac{\mathrm{d}\phi}{\mathrm{d}z} \right)_{z=d/2, \, \phi = \phi_{l1}} = 2 \, W_{\mathrm{a}1} (\phi_{01} - \phi_{d1}) \tag{5}$$

$$k_{22} \left(\frac{\mathrm{d}\phi}{\mathrm{d}z} \right)_{z = -d/2, \, \phi^{=} - \phi_{d2}} = 2 \, W_{\mathrm{a2}}(\phi_{02} - \phi_{d2}). \tag{6}$$

 ϕ_{01} and ϕ_{02} are related to the experimentally measured zero-field twist angles ϕ'_{01} and ϕ'_{02} via the torque balance equations for no applied field:

$$k_{22}\left(\frac{\phi'_{01}+\phi'_{02}}{d}\right) = 2 W_{a1}(\phi_{01}-\phi'_{01})$$
(7)

$$k_{22}\left(\frac{\phi'_{01}+\phi'_{02}}{d}\right) = 2 W_{a2}(\phi_{02}-\phi'_{02}). \tag{8}$$

Hence the twist angle of the liquid crystal director, under the application of an in-plane electric field, as a function of the distance through the cell, can be specified completely using experimentally measurable quantities:

$$z = \xi \sin^{-1} \left[\frac{\phi}{\phi_{d1}} \sin \left(\frac{d}{2\xi} - \frac{\eta}{\xi} \right) \right] + \eta$$
 (9)

or

$$\phi = \phi_{d1} \frac{\sin\left(\frac{z-\eta}{\xi}\right)}{\sin\left(\frac{d}{2\xi} - \frac{\eta}{\xi}\right)}$$
(10)

where

$$\eta = \xi \tan^{-1} \left[B \tan \frac{d}{2\xi} \right]$$
(11)
$$A \frac{k_{22}}{2d} (W_{a2} - W_{a1})(\phi'_{01} + \phi'_{02}) + W_{a1} \phi'_{01} [1 + A W_{a2} + \cos(d/\xi)] - W_{a2} \phi'_{02} [1 + A W_{a1} + \cos(d/\xi)] \right]$$
$$B = \frac{-W_{a2} \phi'_{02} [1 + A W_{a1} + \cos(d/\xi)]}{[2 - A(W_{a1} + W_{a2}) - 2 \cos(d/\xi)] \frac{k_{22}}{2d} (\phi'_{01} + \phi'_{02}) + W_{a1} \phi'_{01} [1 - A W_{a2} - \cos(d/\xi)] + W_{a2} \phi'_{02} [1 - A W_{a1} - \cos(d/\xi)]$$
(12)

and

$$A = \frac{2\xi}{k_{22}} \sin\left(\frac{d}{\xi}\right). \tag{13}$$

This relationship demonstrates that if the dielectric anisotropy $\Delta \varepsilon$ is known, together with the magnitude of the applied electric field, the zero-field twist angles at the substrates, and the cell thickness, then the twist profile of the director through the cell can be generated by choosing values of the constants k_{22} , W_{a1} , and W_{a2} . A multilayer optical theory is used to generate angledependent reflectivity and transmission data from this twist profile. By optimizing the values of the desired parameter, a best fit is obtained to experimental data for several different E-fields.

It is important to know the magnitude of the electric field, the form of which can be determined by solving Laplace's equation for a scalar field between two semiinfinite flat electrodes separated by an in-plane gap g. If there is a potential difference, V, between the two plates then the associated field lines and equi-potentials can be described in an elliptic-cylindrical coordinate frame. Assuming free space and no ionic drift, the electric field defines a hyperbola that can be considered to be of constant value across the electrode gap, except very close to the electrode edges. The magnitude of the field at the centre is given by:

$$\mathbf{E} = \frac{2V}{\pi g} \tag{14}$$

4. Experimental

The cell geometry used in this study is shown in figure 1. The 350 nm thick gold electrodes were evaporated onto the bottom substrate through a mask which provided an electrode gap of 3 mm. Homogeneous alignment of the liquid crystal was obtained by antiparallel aligned rubbed polyimide that was spin-coated onto the sub-strates at 3500 rev s^{-1} for 35 s. The substrates were then baked for $3\frac{1}{2}$ h in an oven at 275°C before being rubbed with a velvet-covered rolling drum in the direction of the electrode edges. Great care was taken not to damage the gold films during rubbing. A cell thickness of approximately 10 µm was obtained using beaded glue. The cell was filled under vacuum with the nematic liquid crystal E7 in the isotropic phase, which was then slowly cooled into the nematic phase to ensure a good monodomain. A 10 kHz a.c. signal was applied across the electrode gap to provide the electric field. The experimental geometry is shown in figure 2. The input polarization of the laser beam is set by the polarizer P1. The beam is directed onto a point on the axis of rotation of a rotating table where the LC cell is positioned in a temperature stabilized environment. The area of the weakly focused (f = 0.5 m lens) beam spot is approximately 0.5 mm² which is significantly smaller than the 3 mm electrode gap. Polarizers P2 and P3 are used to set the polarization of the detected beams.



Figure 2. Schematic of the apparatus used for the FLGM technique. P1, P2, and P3 are polarizers and the cell is positioned on the centre of rotation of the rotating table.

To help in the accuracy of determining the small director distortions, it was felt desirable to explore a large number of guided modes; the data were therefore collected over a wide incident angle range. The scans were recorded in two sections with an angular overlap of 5° and pieced together, the beam spot always sampling the same point in the liquid crystal monodomain.

Once a fit to multilayer optical theory for the director profile in zero-field is obtained it can be used to model the reflectivity and transmission at a fixed angle of incidence as the cell is rotated about a plane normal to the incidence plane (figure 3). This information gives the expected change in optical signal for a given twist of the cell. A suitable azimuthal angle for the cell can then be chosen in which there is a large change in signal for a small variation in twist, and it is in this cell position that the electric field experiments are conducted. The results of the modelling showed that the polarizationconversion signal in transmission is especially sensitive to changes in twist if a suitable azimuthal angle of the cell is chosen. For this reason the transmission signal $T_{\rm ps}$ was chosen to monitor the response of the cell under the application of the electric field.

To model the optical response of the electric field distorted director profile, the liquid crystal is broken into



Figure 3. Model of the effect on the transmitted polarization conversion signal T_{sp} of an azimuthal twist of the cell for fixed angles of incidence θ upon the liquid crystal layer within the glass prism.

100 layers. This ensures that the modelled deformation is a smooth function on the scale of the wavelength of light. Careful fitting of the transmitted polarization conversion signal, T_{ps} , yields both the twist elastic constant k_{22} and the anchoring energies at each substrate, W_{a1} and W_{a2} .

5. Results

Figures 4 and 5 show typical fits to angle-dependent reflectivity and transmission data. Figure 4 illustrates a fit to the R_{ss} signal, and figure 5 illustrates a fit to the T_{ps} signal where the data points are shown as crosses and the theoretical fit as a solid line. The model used to fit these two sets comprised a small twist through the cell of 2.4° with tilt angles at the two substrates of 88.8° and 89.9° (90° is in the substrate plane). The cell thickness was found to be 9.1 µm and the optical permittivities of the LC for an incident wavelength of 632.8 nm at 23.5°C were $\varepsilon_{\parallel} = 2.282$ and $\varepsilon_{\perp} = 2.995$. To obtain a good fit to the field-applied data it was necessary



Figure 4. A typical fit (solid line) to angle-dependent reflectivity data (crosses) with zero-field applied for s-polarized light incident and s-polarized light detected.



Figure 5. A typical fit (solid line) to angle-dependent transmission data (crosses) with zero-field applied for p-polarized light incident and s-polarized light detected.

in the modelling to set the electrode edges twisted away from the alignment direction on the bottom substrate by 1.1°. The T_{ps} signal was found to be very sensitive to small changes in twist, and the fits to this signal as a function of incident angle for several values of in-plane field are shown in figure 6 using a dielectric anisotropy $\Delta \varepsilon = 14.1$ [13]; again the data points are shown as crosses and the theory as a solid line. It should be noted that the fields being used to generate these changes in twist profile are extremely small, the maximum voltage being applied across the 3 mm gap corresponding to an electric field magnitude of less than $3.2 \times 10^{-2} \text{ V} \text{ }\mu\text{m}^{-1}$. Figure 7 shows the comparison between theory and experiment for fixed angles of incidence (θ) , again using $\Delta \varepsilon = 14.1$. The shape of the twist profile used to fit the data is shown in figure 8 for different electric field strengths. The largest twist in the cell occurs, as expected, in the bulk, with the maximum displacement corresponding to 0.5°.



Figure 6. The effect of an in-plane a.c. field (10, 30, 50, 70, 90, 110, 130, 150 V rms across a 3 mm gap) on the transmission signal T_{ps} . The experimental data are shown as crosses and the theory as a solid line.



Figure 7. Variation of the transmission signal T_{ps} with in-plane electric field for fixed angles of incidence θ upon the liquid crystal layer within the glass prism.



Figure 8. Variation of the twist profile spatially through the cell with the application of increasing in-plane fields (maximum field is 150 V rms across the 3 mm gap).

These fits converged to give the following parameters at room temperature (23.5°C) for E7 on rubbed polyimide: $k_{22} = (6.50 \pm 0.05) \times 10^{-12}$ N, and $W_{a1} = W_{a2} = (2.9 \pm 0.2) \times 10^{-5}$ J m⁻². The value of the twist elastic constant obtained here is in very good agreement with that obtained from light scattering experiments [14], and the torsional anchoring energies are of the same magnitude as those reported [15, 16] for alignment on rubbed polymer films. W_{a1} and W_{a2} were found to be equal-valued although they were not constrained to be so while fitting the data to theory.

6. Conclusions

In this experiment a novel optical guided mode procedure, the fully-leaky guided mode technique, has been used to examine a conventional, homogeneously aligned nematic cell. The sensitivity to the director profile of this technique has been proven to be ideal for the study of very small variations in twist, paving the way for a whole new approach to the examination of real commercial liquid crystal cells. Nematic director deformations have been brought about by the application of very weak a.c. fields within the plane of the substrate. From the fits to the angle-dependent optical response of the cell, values for the twist elastic constant k_{22} and the torsional anchoring energies have been determined and are in good agreement with published results. The absence of a true Fréedericksz-style transition in the observed response of the liquid crystal to the applied electric field is wholly in keeping with a small zero-field distortion of the liquid crystal directors, coupled with a finite anchoring strength.

In the treatment of the data a single value for $\Delta \varepsilon = 14.1$ for E7 was taken from the literature [13]. If the data are re-analysed using different values of this parameter, then with appropriate amendments to the parameters W_{a1} , W_{a2} and k_{22} , equally good fits may be obtained for the

series of data sets. A 10% increase in $\Delta \varepsilon$ ($\Delta \varepsilon = 15.5$) leads to $k_{22} = 7.4 \times 10^{-12}$ N with $W_{a1} = W_{a2} = 2.2 \times 10^{-5}$ J m⁻² and a 10% reduction in $\Delta \varepsilon$ ($\Delta \varepsilon = 12.7$) gives $k_{22} = 5.7 \times 10^{-12}$ N with $W_{a1} = W_{a2} = 5.0 \times 10^{-5}$ J m⁻². Thus when using this procedure it is essential that the dielectric anisotropy is determined accurately for the consequential accurate determination of k_{22} and W_a .

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