

Modelling the Electro-Optic Properties of Liquid Crystals

Alastair R. MacGregor

Submitted for the degree of
PhD

Department of Physics
University of Edinburgh

1989



Acknowledgements

I wish to express my thanks to all those who have contributed in any way to this work. Particular thanks must go to my supervisors David Vass, Dick Dougal and Bill Crossland (S.T.C. Technology Limited) who have each helped me greatly by their guidance and encouragement. I am very grateful to Dick Sillitto who has been an inspiration to me and an unofficial supervisor. I have appreciated the freedom which the University of Edinburgh and S.T.C. Technology Limited have given to me to develop this project and hope that they feel that it has been as worthwhile as I do. My appreciation extends to all the members of the Applied Optics Group at the University of Edinburgh and of the Liquid Crystal Technologies Group at S.T.C. Technology Limited who have each contributed, in their own way, to the atmosphere in which this work was carried out. Thanks are also due to Andrew Garrie for general technical assistance, to Peter Tuffy and John Allen (Department of Geology, University of St.Andrews) for help with preparing the photographic results presented in this thesis and to John Murison (Edinburgh University Computing Service) for help with producing the grey scale plots in chapter 3. Many thanks are due to DGV, RCD and RMS for proof reading this thesis and the papers I have written over the last three years. Finally, thanks are due to the Science and Engineering Research Council and to S.T.C. Technology Limited for funding this work.

I am grateful to all my family and friends in Edinburgh, St.Andrews and elsewhere who have made the last three years both enjoyable and interesting. Most of all I would like to thank my wife, Lisa, whose love and support, through good and bad times, have been invaluable. I dedicate this thesis to her.

Declaration

I declare that the composition of this thesis, and all the work described within it, was carried out by me, except where otherwise acknowledged.

To Lisa

Prologue

Poets say science takes away from the beauty of the stars — mere globs of gas atoms. Nothing is 'mere'. I too can see the stars on a desert night, and feel them. But do I see less or more? The vastness of the heavens stretches my imagination — stuck on this carousel, my little eye can catch one-million-year old light ... Or see them [the stars] with the greater eye of Palomar, rushing all apart from some common starting point when they were perhaps all together. What is the pattern, or the meaning, or the why? It does not do harm to the mystery to know a little about it. For far more marvellous is the truth than any artists of the past imagined! Why do the poets of the present not speak of it?

Richard Feynman

Abstract

Liquid crystals (LCs) have been recognised as a phase of matter intermediate between solid and liquid for about 100 years. During this time a large variety of mesophases have been discovered but it is only recently that their physics have begun to be understood. However if LCs are to continue to compete successfully in the displays market an improved understanding of their electro-optic properties must be gained. This thesis describes work carried out on two different types of LC: nematic and ferroelectric chiral smectic C (SmC^*). In the former the molecules are orientationally ordered and randomly positioned while in the latter they are orientationally ordered and arranged in layers. The local mean molecular orientation is called the director and defines the uniaxial optic axis in both types of LC.

In a nematic guest-host (NGH) LC an anisotropically absorbing dye is dissolved in the LC and the dye molecules align so that their maximum absorption axis is parallel to the director. When an electric field is applied to a cell containing NGHLC the molecules tend to rotate, because of their dielectric anisotropy, and alter the cell's transmittance. Previous attempts to model the change in optical transmittance with voltage have assumed that the LC and dye molecules are perfectly aligned with the director. In this work the disorder of the molecules about the director is taken into account and the overall agreement between theory and experiment is improved considerably.

A method of calculating how the SmC^* director configuration and layer orientation vary with voltage is presented. This method is tested by calculating the transmittance of a $7\mu\text{m}$ thick SmC^* LC cell for different azimuthal orientations of the cell between crossed polarisers. It is shown that the theoretical and measured orientations which give minimum transmittance are in good agreement. It is also shown that the computed average director tilt angle is consistent with the conoscopic measurements performed with a polarising microscope.

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Chapter 1

Introduction: Liquid Crystals and Their Properties

1.1 Liquid Crystalline Phases

Condensed matter is usually thought of as existing in one of two states: solid or liquid. In a solid the atoms or molecules have fixed relative positions and, if they are anisotropic in shape, fixed relative orientations. The degree of atomic or molecular order can vary enormously within the solid state, for example from virtually perfectly regular ordering in a sodium chloride crystal, through the orientational ordering of polymer chains in nylon to the random atomic distributions in amorphous silicon or glass. However in all of these materials the atomic or molecular positions and orientations are essentially fixed. By contrast in common liquids the atoms or molecules are completely disordered and liquids are both positionally and orientationally isotropic.

Liquid crystals (LCs) combine some of the properties of solids with some of the properties of liquids and are said to form mesophases i.e. phases in between the solid and liquid phases. In all LCs the molecules are orientationally ordered to some degree and in some LCs the molecules are positionally ordered as well.

The degree of orientational and positional ordering of the molecules forms the basis of the classification system used to distinguish between different kinds of LC phases. Despite the molecular ordering which occurs in LCs they are liquids and will flow, albeit with anisotropic viscosity coefficients. Before describing some of the physical properties of liquid crystalline materials the classification system of LCs is explained so that the LC phases considered in this thesis may be seen in the context of the whole range of mesophases which exist.

There are two major classes of LCs: lyotropic and thermotropic. Lyotropic LC phases are formed within certain ranges of concentration when a liquid is absorbed into an organic material. A typical example is the water-soap system. Soaps are the salts of fatty acids and consist of positive cations (usually Na^+ or K^+) and negative anions (of the type $\text{CH}_3-[\text{CH}_2]_{n-2}-\text{CO}_2^-$, with n in the range 12–20) [1, page 5]. Each anion has a long non-polar tail (the carbon chain) which avoids the water molecules and a polar end (the CO_2^- group) which tends to be in close contact with the water molecules. These conflicting requirements cannot be satisfied by a single molecule but they can be satisfied by, for example, a rod-like cluster of molecules such as that shown in figure 1.1. If the ratio of concentration of water to soap is in the right range the rod-like clusters tend to line up with each other and form an anisotropic mesophase. Altering the concentration ratio can bring about other kinds of lyotropic mesophase. No further consideration is given to lyotropic LC systems in this thesis.

Thermotropic LCs (TLCs), in contrast to lyotropic LCs, can occur in pure materials and form their LC phases within certain temperature ranges rather than concentration ranges. TLCs may be either of high molecular mass (polymers) or of low molecular mass (monomers). A review of polymeric LCs is given in reference [2] and they will not be discussed further. Monomeric TLCs are classified as shown in figure 1.2. Nematic LCs have orientational ordering only (see figure 1.3) whereas smectic LCs also have varying degrees of positional ordering. A complete description of all the different smectic phases is given in reference [3]

and figure 1.3 shows the type of ordering which occurs in the smectic A (SmA) and smectic C (SmC) phases. In each of the three phases the local average molecular orientation is called the director and is denoted by the unit vector $\mathbf{n}$. In the two smectic phases an additional unit vector $\mathbf{k}$ defines the direction of the smectic layer normal. $\mathbf{k}$ is parallel to $\mathbf{n}$ in the SmA phase but is rotated by an angle θ from $\mathbf{n}$ in the SmC phase. A further smectic phase, the chiral smectic C (SmC*) phase, is similar to the SmC phase but the $\mathbf{n}$ -director precesses about the layer normal, $\mathbf{k}$, from layer to layer (see figure 4.1, section 4.1). All the work described in this thesis concerns the nematic and SmC* LC phases and the way in which their anisotropies can be used to produce electro-optic light modulators.

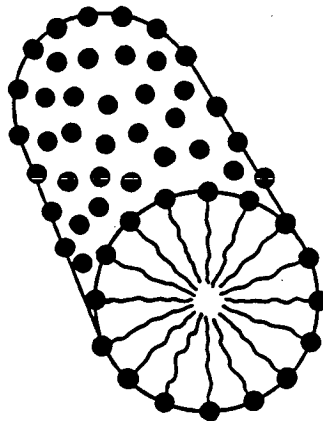


Figure 1.1: A rod-like cluster of soap anions formed when a high concentration of soap is dissolved in water. The dots represent the hydrophilic CO_2^- group and the tails represent the hydrophobic carbon chain of the anion. A lyotropic mesophase is formed when there is a sufficiently high concentration of rods that they align with each other.

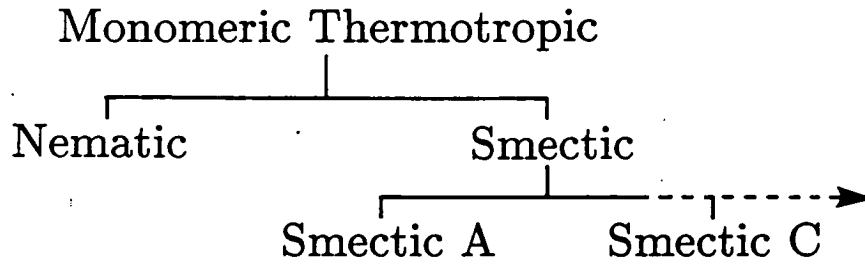


Figure 1.2: Classification of monomeric thermotropic LCs. The smectic subgroup is currently divided into a total of eleven mesophases[3].

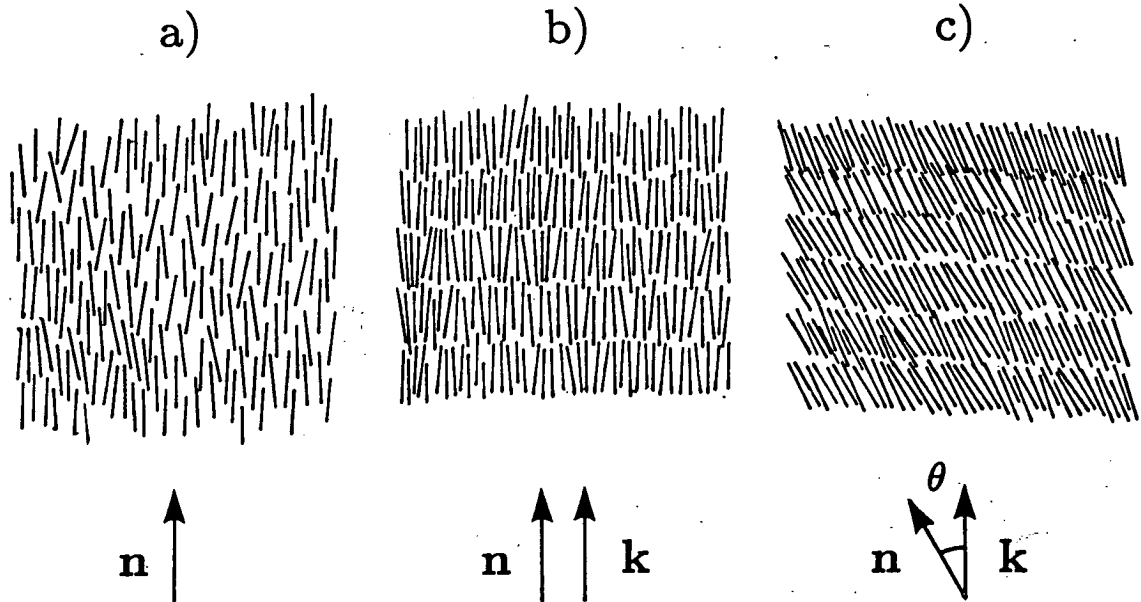


Figure 1.3: Schematic diagram showing the structure of the a) nematic, b) smectic A and c) smectic C phases. In each of the phases the molecules are orientationally ordered with the local mean molecular orientation being defined by the director $\mathbf{n}$. The molecules in the nematic phase are positionally disordered and in the smectic phases are arranged in layers. In the smectic A phase the layer normal, denoted by the vector $\mathbf{k}$, is parallel to the director and in the smectic C phase the layer normal is at an angle θ to the director.

1.2 Anisotropic Properties of LCs

1.2.1 Refractive Index

Both of the LC phases considered in this thesis (nematic and SmC*) are optically uniaxial with the optic axis parallel to the $\mathbf{n}$ -director . The extraordinary and ordinary refractive indices, n_e and n_o , are associated with light polarised parallel and perpendicular to the $\mathbf{n}$ -director respectively. Typically the birefringence Δn , given by

$$\Delta n = n_e - n_o, \quad (1.1)$$

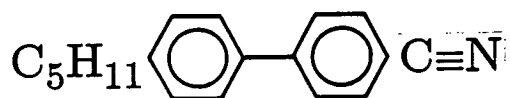
is in the range 0.15–0.2 for both the nematic and the SmC* phases. Δn is large because of the highly anisotropic polarisability of the molecules (see figure 1.4): the delocalised electron clouds of the phenyl rings can be spread out much more easily along the carbon chain than perpendicular to it.

1.2.2 Dielectric Permittivity

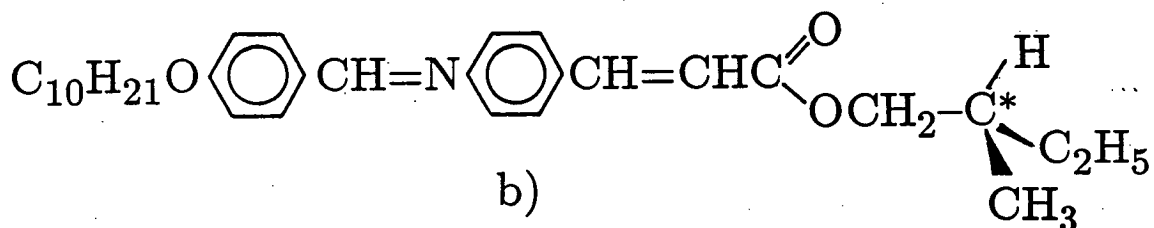
The low-frequency analogue of the birefringence, the dielectric anisotropy $\Delta\epsilon$, is also non-zero. $\Delta\epsilon$ is defined by

$$\Delta\epsilon = \epsilon_{\parallel} - \epsilon_{\perp} \quad (1.2)$$

where $\epsilon_{\parallel}$ and $\epsilon_{\perp}$ are the dielectric permittivities parallel and perpendicular to the $\mathbf{n}$ -director . Most nematic LCs have a large positive dielectric anisotropy ($\Delta\epsilon \sim 10 - 15$) though some have a negative dielectric anisotropy. In both cases this is caused primarily by permanent dipoles within the molecules. SmC* LCs usually have a small negative dielectric anisotropy ($\Delta\epsilon \sim -1$). The sign of the dielectric anisotropy is important in electro-optic devices because it determines whether the molecules tend to rotate so that they are parallel ($\Delta\epsilon > 0$) or perpendicular ($\Delta\epsilon < 0$) to the electric field lines.



a)



b)

Figure 1.4: Chemical formulae of typical a) nematic and b) SmC* LC molecules. The molecules depicted are a) 4-cyano-4'-pentylbiphenyl and b) (S)-4-n-decyloxybenzylideneamino-2'-methyl butyl cinnamate (DOBAMBC). The * on the carbon atom on the DOBAMBC molecule indicates the chiral centre of the molecule i.e. the part of the molecule which has a handedness. The COO group in DOBAMBC produces the transverse dipole moment.

1.2.3 Orientational Elasticity

In the absence of any other constraints the director in a nematic LC will have the same orientation everywhere and in a SmC* LC will take up the configuration described in section 1.1 and illustrated in figure 4.1. Any distortions of these director configurations will increase the elastic free energy of the LC. In both nematic and SmC* LCs it is possible to define a set of basic, linearly independent director orientational distortions and to describe an arbitrary distortion of the director configuration as a linear combination of these basic distortions.

1.2.4 Spontaneous Polarisation

SmC* LC molecules exhibit a spontaneous polarisation, that is they are ferroelectric. For this to be so the molecules must have a transverse dipole moment (in DOBAMBC this is associated with the COO group shown in figure 1.4), be tilted with respect to the smectic layer normal and be chiral [4]. If we represent the chiral group (a carbon atom joined to four different chemical groups as in figure 1.4) as an uneven tripod [4] then figure 1.5 illustrates the tendency of the molecules to tilt in one direction so that their dipole moments tend to line up. The resultant spontaneous polarisation, P_s , is a measure of the strength of the dipole moments. In reality the molecules are spinning rapidly but the preferred tilt direction is the most energetically favoured position.

1.3 Thesis Outline

The work described in this thesis falls into several well-defined sections. In each of them an attempt has been made to elucidate the electro-optic properties of a particular type of LC cell by a combination of experimental, theoretical and

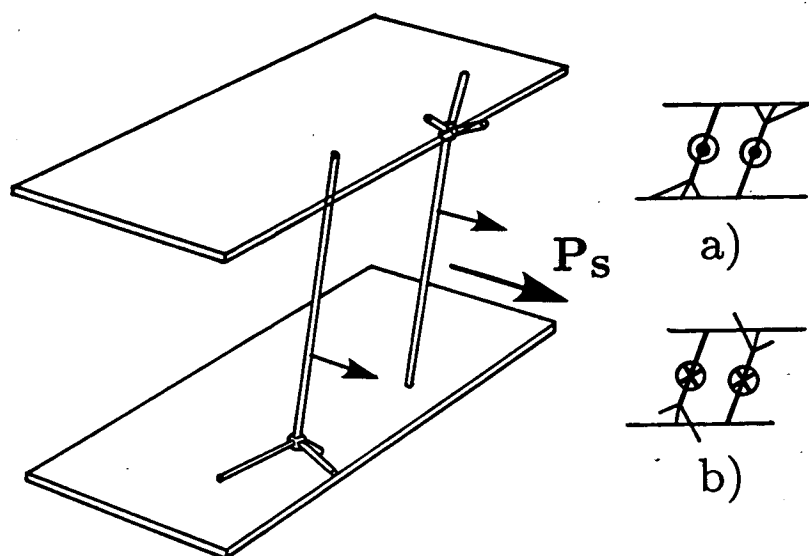


Figure 1.5: Schematic arrangement of molecules in the SmC* phase. Due to the chiral centre, depicted by the uneven tripod, the molecules prefer orientation a) to orientation b) and the molecular dipole moments lie in the same direction producing the spontaneous polarisation P_s .

mathematical modelling techniques. Rather than presenting my conclusions in a general way at the end of this thesis I have listed them at the end of each chapter so that they may be seen in context and their correct perspective.

Chapter 2 describes the technique developed by the author of modelling the optical properties of twisted nematic guest–host LC cells. Equations describing the deformation of a twisted nematic liquid crystal in an electric field in terms of the n -director orientation have been derived by Deuling [5]. In addition Berreman [6] has developed a method of describing the optical properties of such a cell. In this chapter their model has been extended to take account of the degree of orientational disorder of the liquid crystal molecules. An electrical equivalent circuit of the cell is then introduced along with a method of computing the liquid crystal capacitance so that the fraction of the cell voltage appearing across the liquid crystal may be computed. Finally a comparison is made between the experimentally measured light transmission and that predicted by the theory with and without the molecular disorder correction. The overall agreement between theory and experiment is improved considerably when the molecular disorder correction is included.

Conoscopy is one of the techniques used to examine SmC^* LCs in chapters 4 and 5. In chapter 3 a model is presented for computing the conoscopic figures produced by a uniformly oriented liquid crystal (LC) in a thin cell observed with a polarising microscope. The method takes account of refraction and primary reflection at each interface within the cell but neglects multiple reflections. It is shown that the form of the isochromes in the figures is qualitatively given by the intersections of Bertin's surfaces with the LC surface but that refraction also influences the form of the isochromes. Examples of calculated conoscopic figures are presented including the "symmetric flash figure" and the optic–normal figure. The way in which these are altered by small changes in the optic–axis orientation is demonstrated. To complete the model the polarising effect of the microscope condenser and objective lens systems is estimated by calculating the Fresnel

coefficients for a model lens system; the effect on the conoscopic figures is noted. Finally the director tilt in a $7\mu\text{m}$ SmC* LC cell is determined by comparing an experimentally measured figure with a set of calculated figures.

In chapter 4 the general method developed for computing the optical properties of a SmC* LC cell is presented. Previous theoretical and experimental studies of ferroelectric SmC* LCs concentrated on very thin (approximately $2\mu\text{m}$) devices which are difficult to build accurately. In this chapter a formalism is presented, based on a uniformly tilted smectic layer configuration, for computing the director orientation in a cell containing SmC* LC. This formalism is applied to thicker, more easily constructed, LC cells and allows for interactions within and between the smectic layers which have not been considered in previous studies. Results of the director orientation calculations are presented and used in a formalism developed by Berreman [6] to compute the transmittance of a $7\mu\text{m}$ thick cell for different azimuthal orientations of the cell between crossed polarisers. It is shown that the theoretical and measured orientations which give minimum transmittance are in good agreement. Finally it is shown that the computed average-director-tilt angle is consistent with the conoscopic measurements described in chapter 3.

Finally, in chapter 5, the recently discovered^e _{χ} symmetric chevron smectic layer structure is incorporated into the model described in chapter 4. This revised model is also shown to be consistent with the experimental observations cited in chapter 4. However the chevron layer structure enables a physical understanding to be gained of the interactions between the LC and the LC alignment layer and also explains the reason why there is such a large difference between the extinction orientations of the relaxed states of thin ($\sim 2\mu\text{m}$) and thick ($\sim 7\mu\text{m}$) SmC* LC cells between crossed polarisers.

Chapter 2

Modelling the Optical Properties of Twisted Nematic Guest–Host Liquid Crystals

2.1 The Twisted Nematic Guest–Host Liquid Crystal Cell

Nematic liquid crystals (LCs), including nematic guest-host LCs, are characterised by orientational order and positional disorder of their molecules. The director, a unit vector $\mathbf{n}$, is defined as the local mean molecular orientation. This direction coincides with the major axis of the dielectric ellipsoid and the optic axis defining the material's birefringent properties. In a guest–host LC a small quantity of dichroic dye (guest) with the properties shown in figure 2.1, is dissolved in a nematic LC (host). The dye is chosen so that its maximum absorption axis aligns parallel to the director. If the electric field vector of light passing through the guest–host LC is parallel to the long axis of the dye molecules the light is strongly absorbed but if the electric field vector is perpendicular to the long axis the light is absorbed only weakly. A sufficiently small quantity of dye ($\sim 2\%$) is dissolved that the visco-elastic and dielectric properties of the nematic host are virtually unchanged. It will be assumed in the following discussion that

the dye molecules are fully dissolved in the LC and that the solution behaves as a dichroic LC. In particular it will be assumed that the mean orientation and the orientational probability-density-function of the guest and host molecules are the same.

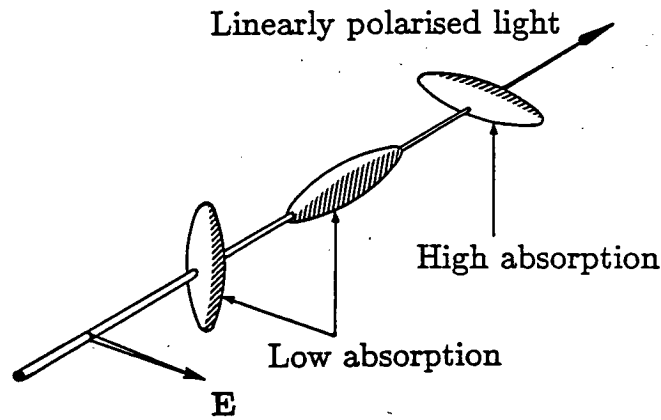


Figure 2.1: Light absorption by a dichroic dye molecule.

In a twisted nematic LC cell the dielectric and optical anisotropies are used to modulate light passing through the cell [7]. Figure 2.2 shows schematically the construction of a typical LC cell. Two glass plates are coated first with (transparent) indium tin oxide (ITO) electrodes and second with a LC aligning layer. Uniform alignment of the LC director parallel to the surface is produced either by a layer of rubbed polymer [8] such as nylon or PVA or by a layer of obliquely evaporated magnesium fluoride (MgF_2) or silicon monoxide (SiO) [9, section 1.5]. In the former method alignment is produced by a combination of geometrical factors and Van der Waals interactions between the LC molecules and the polymer molecules which are aligned by the rubbing process. In the latter method the alignment mechanism is not well understood but is thought to be due to Van der Waals interactions between the aromatic rings in the LC molecules and the crystalline structure of the alignment layer [10]. Both methods produce well-defined alignment of the nematic director. A variety of methods can be used to space the coated glass plates a uniform distance apart including polyester sheet at the edges of the cell and short sections of fibreglass rod or

Material	Thickness (μm)	Area (mm^2)	Dielectric constant
Glass	3.0×10^3	25×25	—
Indium tin oxide	0.05	25×25	—
Magnesium fluoride	0.12	25×25	1.912
Polyester spacer	13	2.5×25	3.8
LC layer	13	25×25	—

Table 2.1: Specification of the LC cell

plastic spheres arbitrarily positioned between the plates. However if the first method is used then care must be taken to avoid bowing of the glass plates.

Oblique evaporation of MgF_2 , at an angle of 30° to the surface normal, was found to give repeatable uniform alignment and was used throughout the work described in this chapter. An alignment-layer thickness of $120 \pm 10nm$ was measured using a Talystep (Rank Taylor Hobson). Polyester spacers, positioned as shown in figure 2.2, were used to space the 3mm thick glass plates. The spacer thickness was measured using a digital micrometer and found to be $13 \pm 1\mu m$. A typical value of the ITO thickness was assumed [16]. Table 2.1 summarises the specification of the LC cell which was built. The empty cell was assembled, with perpendicular alignment directions, in a laminar-flow clean cabinet and was bonded together along the sides with spacers using epoxy resin. A drop of the Roche LC mixture 1263 was placed, using a hypodermic syringe, on one of the open sides of the cell and was allowed to fill the cell by capillary action. After filling, the complete cell was heated to just above the LC clearing point (nematic to isotropic phase-transition temperature: $90^\circ C$ in this case) and allowed to cool slowly to destroy any flow-induced LC alignment [24, chapter 5]. Figure 2.3a shows schematically the uniformly-twisted director configuration which is formed across the cell.

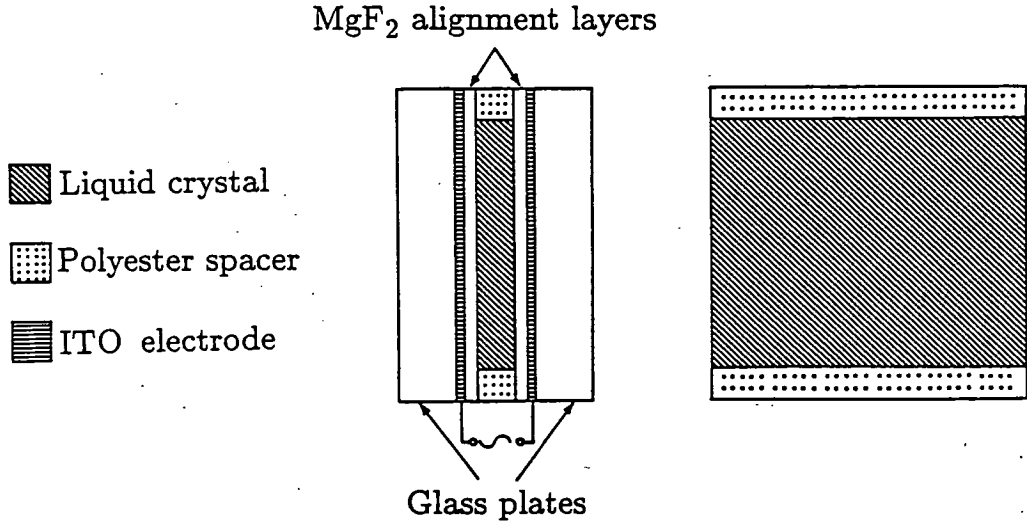


Figure 2.2: A schematic diagram of the LC cell (section and plan views).

Nematic LCs usually have a large positive dielectric anisotropy: for the Roche LC mixture 1263, $\Delta\epsilon = \epsilon_{\parallel} - \epsilon_{\perp} = 8.5$. In the absence of other constraints the LC molecules will reorientate in an electric field until the director is parallel to the electric field direction. In a twisted nematic LC cell director reorientation is hindered by two factors: the LC director at the cell surfaces is fixed in orientation to a first approximation [11]; and elastic forces (see section 2.2) oppose local changes in director orientation. As a result the LC director in the center of the cell reorientates most. It is widely known that there is a well-defined threshold voltage, U_T , below which no reorientation occurs [22]. Figure 2.3b shows the director configuration, calculated using the technique described in section 2.2, when a voltage twice the threshold voltage is applied across the ITO electrodes. This director reorientation forms the basis of many of the electro-optic effects commonly used in LCs [12] and is described in more detail below.

Below the threshold voltage linearly polarised light normally incident on the cell, polarised parallel to the front-face director, is waveguided along the uniformly twisted structure and is strongly absorbed by the guest dye molecules. The wave

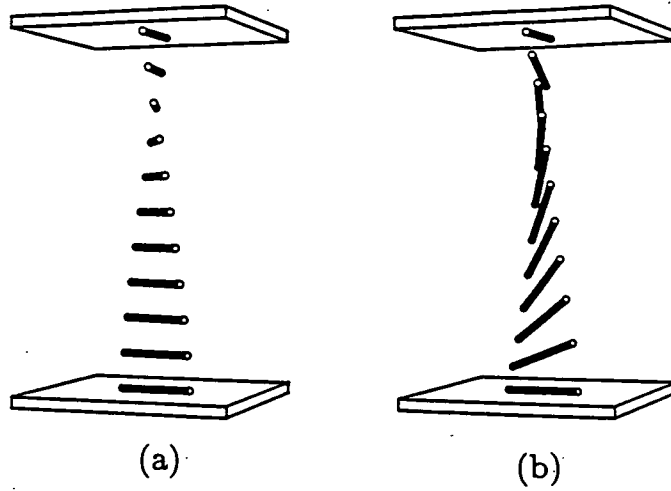


Figure 2.3: Twisted nematic director configuration with applied voltage (a) $U \leq U_T$ and (b) $U = 2U_T$.

guiding only occurs [7] if

$$d\Delta n > 2\lambda \quad (2.1)$$

where d is the LC thickness, Δn is the LC birefringence and λ is the wavelength of the light. However, for voltages above the threshold, the LC and dye molecules tilt so that they are no longer parallel to the cell walls. The cell transmittance increases with voltage as the waveguiding breaks down (because the effective birefringence is lowered) and the absorption by the dye molecules decreases. The LC configuration described above has been employed in a reflection-mode electronically-addressed LC spatial light modulator [13] which has been used as a Fourier-plane filter in a coherent optical processing system. The reason for using a twisted instead of an untwisted cell is the sharper threshold observed for the transmission against voltage curve for the twisted cell [14].

In previous work on the optical properties of twisted nematics [15,16] the LC molecules were all assumed to lie parallel to the director. However the director specifies only the mean molecular orientation and indicates nothing about the orientational distribution about the mean. Orientational fluctuations in LCs

occur at many different frequencies [24, section 5.4] (typically in the range MHz to GHz) and on many different scales [18] (from individual molecular orientational fluctuations to macroscopic director orientational fluctuations). In this chapter it is assumed that the disorder may be described completely in terms of director fluctuations. A director probability-density-function in orientation is introduced and its effect on the calculated optical properties of the twisted nematic guest-host LC cell is investigated. It is found that the agreement between the measured and calculated cell transmittances is improved greatly by the inclusion of the director fluctuations.

2.2 Calculating the Minimum-Energy Director Configuration

Frank [19] has shown that an arbitrary elastic deformation of a nematic LC may be uniquely described as a linear combination of splay, twist and bend distortions. These distortions have associated elastic constants k_{11} , k_{22} and k_{33} . For a cell of thickness L subject to electric field $\mathbf{E}$ at constant temperature and pressure the Gibbs' free energy per unit area of the cell is

$$G = \frac{1}{2} \int_0^L [k_{11}(\nabla \cdot \mathbf{n})^2 + k_{22}(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + k_{33}(\mathbf{n} \times \nabla \times \mathbf{n})^2 - \mathbf{D} \cdot \mathbf{E}] dz. \quad (2.2)$$

The first, second and third terms in equation 2.2 describe the energy per unit area associated with the splay, twist and bend director distortions shown schematically in figure 2.4, and the last term is the dielectric free energy per unit area. Equation 2.2 is valid for sinusoidal electric fields provided that the r.m.s. field amplitude is used and that the field frequency is very much greater than the LC switching frequency. The director orientation is described in terms of the tilt (θ) and twist (ϕ) angles defined in figure 2.5. In terms of the tilt and twist angles

equation 2.2 is

$$G = \frac{1}{2} \int_0^L \left[(k_{11} \cos^2 \theta + k_{33} \sin^2 \theta) \left(\frac{\partial \theta}{\partial z} \right)^2 + (k_{22} \cos^2 \theta + k_{33} \sin^2 \theta) \cos^2 \theta \left(\frac{\partial \phi}{\partial z} \right)^2 \right] dz - \frac{1}{2} \left(\frac{D_z^2}{\epsilon_o} \right) \int_0^L \frac{dz}{(\epsilon_{\parallel} \sin^2 \theta + \epsilon_{\perp} \cos^2 \theta)}. \quad (2.3)$$

The minimum-energy director configuration is found by minimising the right-hand side of equation 2.3 using the calculus of variations. However the equations derived by Deuling [15] and Montgomery [22] are difficult to solve numerically for voltages above $\sim 4V$ r.m.s. because they have an infinite singularity in them (see appendix A) corresponding to the situation in which the molecules in the centre of the cell are perpendicular to the cell walls. Welford and Sambles [20] have found an elegant solution to a similar problem in the equations describing planar (untwisted) nematic cells which avoids the problem by using a change of variables. Using the same substitution here (see appendix A) to improve the behaviour of the numerical solution, thereby extending the voltage range over which solutions may be evaluated, we have calculated the director orientation through the cell for voltages up to $7V$ r.m.s. for the LC specification given in

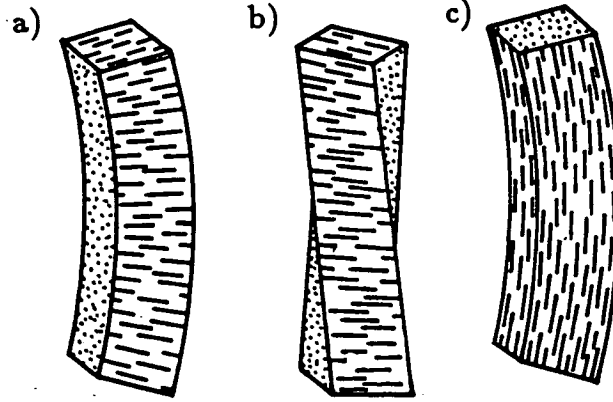


Figure 2.4: Schematic diagram illustrating the three possible modes of distortion of a nematic LC: a) splay, b) twist and c) bend. The increases in free energy associated with these distortions are proportional to the elastic constants k_{11} , k_{22} and k_{33} respectively.

table 2.2. Figure 2.6 shows the calculated tilt and twist configurations across the cell for various values of the r.m.s. voltage.

Splay elastic constant, k_{11}	$14.4 \times 10^{-12} N$
Twist elastic constant, k_{22}	$7.0 \times 10^{-12} N$
Bend elastic constant, k_{33}	$20.0 \times 10^{-12} N$
Parallel dielectric constant, $\epsilon_{ }$	12.3
Perpendicular dielectric constant, $\epsilon_{\perp}$	3.8

Table 2.2: Specification of the Roche LC mixture 1263.

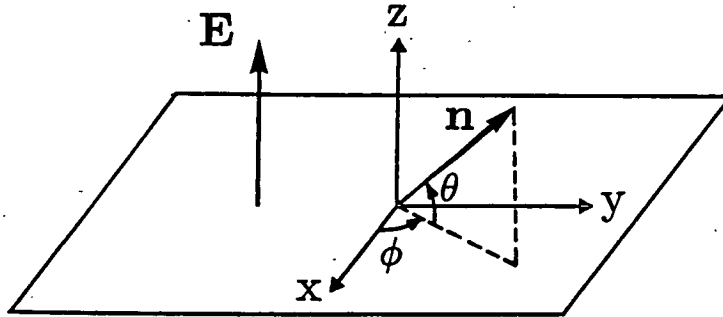


Figure 2.5: Definition of the tilt (θ) and twist (ϕ) angles which define the orientation of the nematic director $\mathbf{n}$.

Of particular interest is the $1.74V$ twist curve which is altered from the threshold voltage twist curve in the opposite sense to the twist change at larger voltages. This “reverse twist” effect is important because it influences the optical transmission at low voltages. While the distortion threshold voltage is $1.46V$ the apparent optical threshold occurs at voltages at least $0.5V$ above this (cf figure 2.11a). The reason for the reverse twist can be seen by considering, in the following simple model, the way in which the distortion energy is partitioned between splay, twist and bend deformations.

The curves in figure 2.6 show that at the threshold voltage the twist angle $\phi(z/L)$

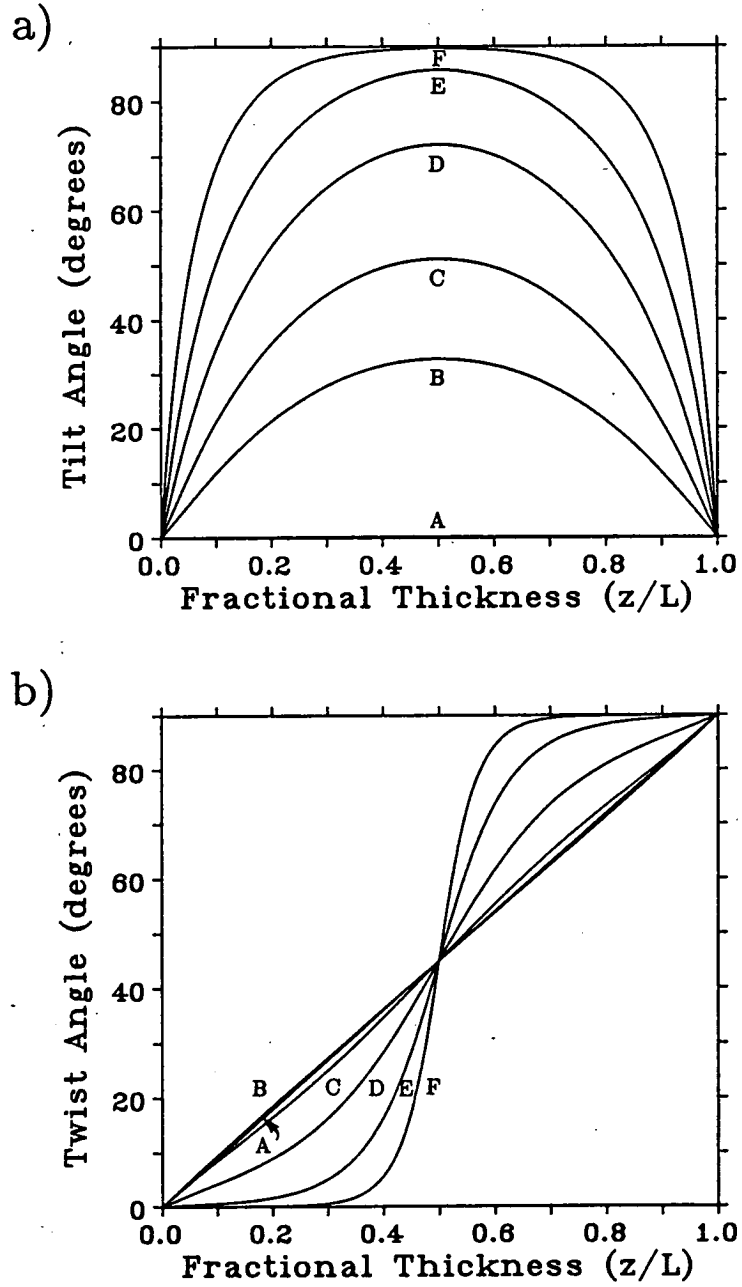


Figure 2.6: Variation of (a) tilt (θ) and (b) twist (ϕ) angles through the LC cell with applied voltages $U = U_T = 1.46V$ (A), $U = 1.74V$ (B), $U = 2.09V$ (C), $U = 2.78V$ (D), $U = 4.17V$ (E) and $U = 6.95V$ (F).

A (deg)	Twist energy	Bend energy	Total energy
-1	6.308	4.199	10.507
0	6.145	4.364	10.509
1	6.013	4.543	10.556

Table 2.3: Twist and bend energies and their sum (arbitrary units) for different distortion amplitudes.

varies linearly with the fractional distance z/L through the cell. At voltages just above threshold the twist angle deviates from this linear relationship and we assume that the twist angle may be approximated by the expression

$$\phi\left(\frac{z}{L}\right) = \frac{\pi}{2}\left(\frac{z}{L}\right) - A \sin\left(\frac{2\pi z}{L}\right) \quad (2.4)$$

where A is the amplitude of the distortion. A positive value of A corresponds to the sense of twist found at large voltages and a negative value of A to reverse twist. The tilt angle was taken as having the actual functional dependence given by the solution to the minimum-free-energy equations. Only the third and fourth terms in equation 2.3, corresponding to the twist and bend energies respectively, are functions of twist angle and therefore vary with A . These twist and bend energies and their sum were computed for various values of A at a voltage of 1.74V between the distortion and optical threshold voltages. Table 2.3 lists these energies in arbitrary units. Although the twist energy is higher for the reverse-twist configuration the bend energy is lower. Summing the twist and bend energies shows that at a voltage of 1.74V r.m.s. the minimum energy configuration occurs for a negative value of A i.e. a reverse twist configuration. As the voltage is increased the energy minimum moves from negative to positive values of A which correspond to twist in the familiar sense.

2.3 LC Cell Optical Properties

A summary of the basic method used to calculate the optical properties of a LC cell is given in this chapter and a fuller description is given in appendix B. The optical properties of the LC cell are uniquely determined by the solution of Maxwell's equations. Berreman [21] showed how the transmitted and reflected electromagnetic fields may be calculated for an anisotropic medium using a 4×4 optical propagation matrix operating on a 4-vector which specifies the transverse electromagnetic field incident on the LC layer. Montgomery [22] extended the method to take account of the isotropic layers in the cell. In practice the solution may be calculated very accurately by careful implementation on a computer. It is found that an efficient way to do this is to divide the LC layer up into slices, approximating the variation in optical properties across each slice by a polynomial fitted to the data using Newton's divided difference formulae. A propagation matrix is then computed for each slice and the matrices are multiplied together to compute the propagation matrix for the whole LC layer. This is more efficient than treating the LC as a single thick slice because the elements of the propagation matrix are power series expansions which converge more rapidly for thin slices than for thick slices. However, the reduction in computation time for thin slices must be weighed against the increase in computation time due to the increased number of slices. Using 1000 slices provides a balance between these considerations.

To describe the optical properties of guest-host liquid crystals it is necessary to take account of the absorption caused by the dichroic dye. The author did this by replacing the real refractive indices in the optical propagation matrix by complex refractive indices whose imaginary components are directly proportional to the absorption coefficients (see appendix B).

Propagation matrices for the cover-glass, ITO and magnesium fluoride layers

are also computed (see appendix B). These matrices are multiplied together, along with the LC layer propagation matrix, so that they operate on the vector describing the incident light wave in the same order that the light traverses the cell layers. Reflected and transmitted electromagnetic fields are computed from the resulting vector. Table 2.4 lists the values of the optical constants used in the calculations.

LC extraordinary refractive index, n_e	1.639
LC ordinary refractive index, n_o	1.500
LC parallel absorption coefficient, $D_{ }$	$0.3940\mu m^{-1}$
LC perpendicular absorption coefficient, $D_{\perp}$	$0.0386\mu m^{-1}$
Magnesium fluoride refractive index	1.383
ITO refractive index	2.0
Glass refractive index	1.54

Table 2.4: Optical constants and cell parameters used in the calculations.

The author found by varying the degree of the polynomial used to fit the change in optical properties from slice to slice that Scheffer's [14] approximation of uniform properties within slices incurs negligible errors. The maximum absolute error in the optical transmission was one part in 10^5 . We also found that the speed of computation could be increased by a factor of forty over Berreman's method if the general form of the slice propagation matrix was multiplied out and used in all subsequent calculations (see appendix B).

2.4 LC Cell Electrical Properties

We shall now determine the relationship between the cell voltage and the voltage applied to the LC layer, using the electrical equivalent circuit shown in figure 2.7.

It is assumed that the electrical properties of each component of the LC cell are uniform in the xy plane (cf figure 2.5). In the equivalent circuit the resistance of an ITO electrode, the LC resistance, the capacitance of a MgF_2 alignment layer, the capacitance of the spacers and the LC capacitance are denoted by R_{ITO} , R_{LC} , C_{MgF_2} , C_{spacer} and C_{LC} respectively.

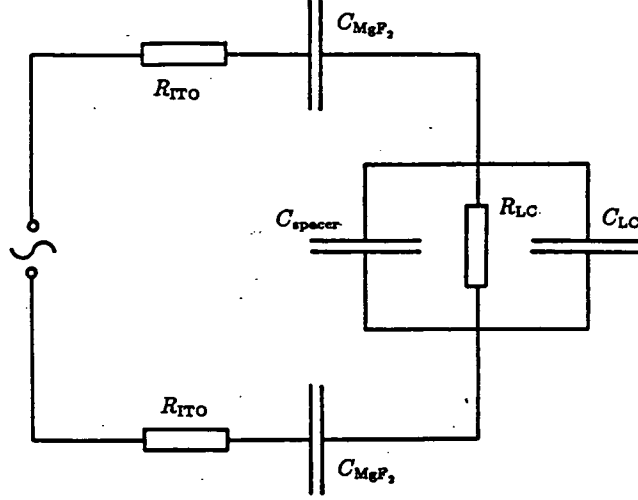


Figure 2.7: Equivalent circuit used to model the LC cell. $R_{ITO} = 400\Omega$, $C_{\text{MgF}_2} = 88\text{nF}$, $C_{\text{spacer}} = 0.32\text{nF}$, $R_{LC} = 2\text{M}\Omega$.

The resistance values required for the equivalent circuit were measured directly using a Beckman 3050 resistance meter and the capacitances of the spacers and the magnesium fluoride layers were calculated for a 1.6kHz sinusoidal voltage signal from their dimensions and dielectric properties (table 2.1). Using the tilt-angle data the capacitance C_{LC} of the LC layer was calculated using

$$\frac{1}{C_{LC}} = \sum_{i=1}^{1000} \frac{1}{C_i} \quad (2.5)$$

where

$$\frac{1}{C_i} = \int_{z_{i-1}}^{z_i} \frac{dz}{\epsilon_o \epsilon(\theta) A_{LC}} \quad (2.6)$$

and C_i is the capacitance of the slice i of thickness $z_i - z_{i-1}$ and area A_{LC} . The

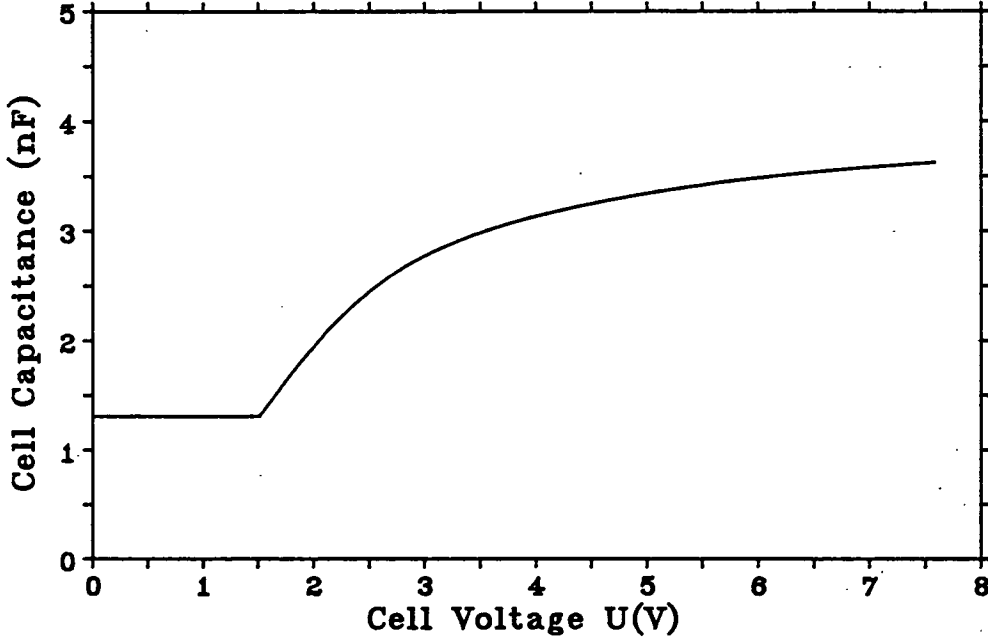


Figure 2.8: Computed capacitance of a $13\mu m$ LC cell.

dielectric function $\epsilon(\theta)$ [15] is given by

$$\epsilon(\theta) = \epsilon_{\parallel} \sin^2 \theta + \epsilon_{\perp} \cos^2 \theta. \quad (2.7)$$

The integral in equation 2.6 was evaluated for each slice of the LC by fitting a polynomial to the tilt angle data for that layer and its neighbours. As in the optical calculation, negligible error was found to be introduced by assuming that the dielectric properties of the layer were uniform across it. Figure 2.8 shows the computed capacitance of a $13\mu m$ LC cell.

With the calculated capacitance substituted into the equivalent circuit, the voltage dropped across the LC could be calculated for a variety of cell voltages. The fraction of the cell voltage appearing across the LC layer varied slowly from 0.964 at the threshold to 0.922 at the maximum voltage. Since the relationship between the voltages dropped across the LC and the cell was known plots could be made of LC cell optical transmittance versus cell voltage.

2.5 Molecular Disorder and LC Properties

2.5.1 Theory

In the preceding discussion the LC molecules were assumed to be parallel to the director. However the director specifies only the local mean molecular orientation and indicates nothing about the degree of orientational order. The order parameter S is a measure of this ordering and is defined by de Gennes [24, page 24] as

$$S = \frac{3}{2} \langle \cos^2 \alpha_l \rangle - \frac{1}{2}. \quad (2.8)$$

In this expression the angle brackets denote the temporal average of the function $\cos^2 \alpha_l$, and α_l is the angle between the (time dependent) molecular orientation and the director. Separate order parameters for the host nematic and guest dye may be defined. However, in the following, as no detailed information was available from the manufacturer, the guest was assumed to be isomorphic with the host and the order parameters equal. For the Roche guest-host LC mixture 1263 at 22°C, $S = 0.77$. It is important to consider the effects of molecular disorder because of the non-linear relationship between molecular orientation and macroscopic optical and dielectric properties. It has been shown [24, section 5.4] that the frequency of the perturbations is of order MHz to GHz so the 1.6kHz voltage signal will not resolve the orientational changes while they will be apparent to the $\sim 10^5$ GHz light signal. Therefore the mean values of the dielectric constants may be used correctly in the director and capacitance calculations. However, in the optical calculations, the local fluctuations in director orientation, resulting from the molecular disorder, must be taken into account. It is assumed that the molecular disorder may be completely described by local fluctuations in director orientation. The optical transmittance of a LC is measured on a timescale much greater than that of the director fluctuations. Therefore the theoretical transmittance should be calculated by taking the mean of the

transmittances evaluated for all possible variations in the director configuration correctly weighted by a probability–density–function in orientation. To do this it is necessary to know the values which the complex refractive indices would have if the LC were perfectly ordered and also the probability–density–function in orientation.

Various models, summarised by Blinov [25, page 22], have been put forward to describe the the local molecular probability–density–function in orientation $P_l(\alpha_l)$. The most sophisticated of these models is due Maier and Saupe [27]. They have derived a form for $P_l(\alpha_l)$ from a model describing the van der Waals forces between molecules. Since the slices considered in the optical calculation are only of order ten molecules thick the local director probability–density–function in orientation was assumed, in accord with [27], to have the form

$$P_l(\alpha_l) = \frac{\exp(\sigma \cos^2 \alpha_l)}{4\pi Z_\sigma} \quad (2.9)$$

where

$$Z_\sigma = \int_0^{\pi/2} \exp(\sigma \cos^2 \alpha_l) \sin \alpha_l d\alpha_l. \quad (2.10)$$

Here σ is a parameter which may be adjusted to vary the distribution–width to take account of the unknown difference between the theoretical situations considered. σ is referred to hereafter as the disorder factor as it is a measure of the width of the orientational probability distribution function. $P_l(\alpha_l)$ was used to describe the orientational ordering in each of the thousand slices of the optical calculation. In practice the value of σ is unknown so the relationship between the measured and perfectly–ordered local refractive indices is also unknown. However the values of the perfectly ordered refractive indices may be estimated using a global probability–density–function in orientation as shown below. Light traversing the LC follows a path much longer than the coherence length of the fluctuations (which is typically several tens of nanometers [24, section 5.4]). Therefore, regardless of the form of the local probability–density–function in orientation, the time variation of the spatial average fluctuation, α , for the path through the LC will be approximately Gaussian

in form. This result follows from the central limit theorem. On this basis we define a global probability–density–function in orientation $p_g(\alpha)$ which describes the fluctuations of α :

$$p_g(\alpha) = \frac{\exp(-\alpha^2/\omega^2)}{4\pi Z_\omega} \quad (2.11)$$

where

$$Z_\omega = \int_0^{\pi/2} \exp(-\alpha^2/\omega^2) \sin \alpha \, d\alpha. \quad (2.12)$$

To find the value of ω we assume that equation 2.8 also holds for the spatial average fluctuation α and its temporal probability–density–function in orientation $p_g(\alpha)$. The expression for $p_g(\alpha)$ is then substituted into equation 2.8 and equation 2.8 is solved for the Gaussian width ω using the bisection method [26, p221]. The value of ω is found to be 0.42 radians.

First we calculate the absorption coefficients associated with the perfectly ordered LC. We assume that each dye molecule has one absorption dipole only, that this is aligned at an angle β with respect to the long molecular axis, and that, in the molecular frame of reference, perpendicular to this axis there is no absorption. The total absorption coefficient, Δ , of the perfectly ordered LC is then given [27] by

$$\Delta = D_{\parallel} + 2D_{\perp} \quad (2.13)$$

where $D_{\parallel}$ and $D_{\perp}$ are the measured absorption coefficients parallel and perpendicular to the director. When the principal absorption axis of the dye molecules is at an angle β to their long axis Saupe and Maier [27] also showed that

$$S = \frac{gN - 1}{(gN + 2)(1 - \frac{3}{2}\sin^2 \beta)} \quad (2.14)$$

where $N = D_{\parallel}/D_{\perp}$ and $g = n_e/n_o$. For the LC material whose specification is given in table 2.4, β is found to be zero. Therefore the principal absorption axis is parallel to the long molecular axis and molecular rotations about this axis do not affect the absorption coefficients. Then, on the basis of the previously stated assumption that the guest dye is isomorphic with host nematic, the parallel absorption coefficient, $\Delta_{\parallel}$, associated with the perfectly ordered LC is given by

the right hand side of equation 2.13, and the perpendicular absorption coefficient, $\Delta_{\perp}$, is zero.

Second, the refractive indices of the ordered structure are calculated using the equation relating the refractive index associated with the wavefront-normal velocity to the instantaneous local orientation of the optic axis [28, page 93]:

$$\frac{1}{\nu_{\alpha}^2} = \frac{\cos^2 \alpha}{\nu_e^2} + \frac{\sin^2 \alpha}{\nu_o^2}. \quad (2.15)$$

If we average over all possible orientations by integrating the expression for ν_{α} , weighted by the probability-density-function in orientation $p_g(\alpha)$, the following implicit, coupled equations are obtained for the perfectly-ordered LC's refractive indices ν_e and ν_o :

$$\begin{aligned} n_e &= \int_{\alpha=0}^{\pi} \int_{\gamma=0}^{2\pi} p_g(\alpha) \nu_{\alpha} \sin \alpha \, d\alpha \, d\gamma \\ &= \frac{\nu_e \nu_o}{4\pi Z_{\omega}} \int_{\alpha=0}^{\pi} \int_{\gamma=0}^{2\pi} \frac{\exp(-\alpha^2/\omega^2) \sin \alpha \, d\alpha \, d\gamma}{\sqrt{\nu_e^2 \sin^2 \alpha + \nu_o^2 \cos^2 \alpha}} \\ &= \frac{\nu_o}{Z_{\omega}} \int_0^{\pi/2} \frac{\exp(-\alpha^2/\omega^2) \sin \alpha \, d\alpha}{\sqrt{1 - K^2 \cos^2 \alpha}}, \end{aligned} \quad (2.16)$$

$$\begin{aligned} n_o &= \frac{\nu_e \nu_o}{4\pi Z_{\omega}} \int_{\alpha=0}^{\pi} \int_{\gamma=0}^{2\pi} \frac{\exp(-\alpha^2/\omega^2) \sin \alpha \, d\alpha \, d\gamma}{\sqrt{\nu_e^2 (\cos^2 \alpha \sin^2 \gamma + \cos^2 \gamma) + \nu_o^2 \sin^2 \alpha \sin^2 \gamma}} \\ &= \frac{\nu_o}{Z_{\omega}} \int_0^{\pi/2} \Psi(K \sin \alpha) \exp(-\alpha^2/\omega^2) \sin \alpha \, d\alpha, \end{aligned} \quad (2.17)$$

where

$$\Psi(x) = 1 + \left(\frac{1}{2}\right)^2 x^2 + \left(\frac{1 \cdot 3}{2 \cdot 4}\right)^2 x^4 + \dots + \left(\frac{(2n-1)!!}{2^n n!}\right)^2 x^{2n} + \dots, \quad (2.18)$$

γ is the azimuthal angle and $K^2 = 1 - \nu_o^2/\nu_e^2$. The function $\Psi(x)$ arises in the context of complete elliptic integrals [29, pages 904-5]. We may find K^2 by dividing equation 2.17 by equation 2.16 (to eliminate ν_o) and using the bisection method. ν_o can then be found from equation 2.16 and ν_e can be calculated from the definition of K^2 . Table 2.5 lists the ordered LC's optical constants.

An alternative method, which avoids the introduction of $p_g(\alpha)$, is described by de Jeu [30, chapter 4, equation 8]. In his method it is necessary to assume that

the electric field strength within the LC is independent of molecular orientation. As de Jeu states, this assumption has no physical basis and is likely to be only approximately true. However the values predicted by de Jeu's model for ν_e and ν_o are 1.666 and 1.485 respectively which are very similar to those contained in table 2.5. The assumptions necessary to justify the model de Jeu describes are thought to be stronger than those necessary to justify the model described above.

2.5.2 Computational Technique

The mean director orientation was computed, using the technique described in section 2.2, at each of 1000 points through the LC layer. This was done for a range of voltages from threshold up to 7V r.m.s. and the results were stored in the form of look-up tables. These results were then used to compute the LC layer capacitance at different voltages as described in section 2.4. The capacitance values were substituted into the LC cell equivalent circuit shown in figure 2.7 to calculate the voltage across the cell corresponding to each voltage across the LC. Cell voltage is a much more useful quantity than LC voltage in this case because the optical properties predicted may be compared directly with experimental transmission measurements.

First the transmission was computed, at each voltage, using the measured val-

Parallel absorption coefficient, $\Delta_{\parallel}$	$0.4712\mu m^{-1}$
Perpendicular absorption coefficient, $\Delta_{\perp}$	0
Extraordinary refractive index, ν_e	1.671
Ordinary refractive index, ν_o	1.488

Table 2.5: Perfectly-ordered LC optical constants

ues of the complex refractive indices, assuming the director to be fixed in its mean orientation, as described in section 2.3. Secondly the transmission was computed, taking account of the director fluctuations, in the following way.

Within each of the 1000 slices of the LC layer, the optic axis was assumed to have probability-density-function in orientation $P_l(\alpha_l)$ about the mean calculated above. A random number generator [31] with probability-density-function $P_l(\alpha_l)$ was used to select a set of orientational deviations from the mean, one for each slice. The tilt and twist angles were then calculated for each slice through the LC layer and, using the computed refractive indices ν_e and ν_o , the cell's transmission was computed. Another set of orientational deviations from the mean was selected randomly and the cell's transmission computed. The transmission of the cell for further random configurations was computed until the successive mean transmissions varied by less than 2%. Typically this condition was satisfied by taking the mean transmission from one hundred configurations.

The width of the local probability density function i.e. the value of the disorder factor σ , was varied to obtain a best fit with the transmission against cell-voltage curve measured experimentally.

2.6 Experimental Measurements

A schematic diagram of the optical bench used for all experimental measurements is shown in figure 2.9. Light from a 5mW HeNe laser was passed through a spatial filter and collimated by a lens. The beam diameter was reduced to 3mm by an aperture and the light passed through a high quality sheet polariser into the LC cell. Light transmitted by the cell was analysed by a second polariser and focussed onto a photodiode (RS 7900 with integrated amplifier) by the second lens.

Voltage control for the LC cell was provided by the custom built amplifier and stepper-motor-controlled voltage divider ($5k\Omega$ variable resistor) shown in figure 2.10. The high input-impedance FET operational amplifier 3140 amplifies the input sinusoidal signal and the second stage acts as an inverting subtractor to remove any d.c. component from the amplified signal. A subtractor is included as any d.c. component would cause electrolytic decomposition of the LC. A BBC-B microcomputer controls the position of the sliding contact on the $5k\Omega$ variable resistor (figure 2.10) with a stepping motor and this sets the voltage across the LC cell. The resistance in parallel with the LC cell could be set to any of 480 values between 0 and $5k\Omega$. Output from the photodiode (figure 2.9) was fed through a signal conditioner to the BBC-B.

Sets of measurements of the transmission of the LC were made by increasing the LC voltage from zero to 20V peak-to-peak in steps of about $42mV$ and recording the light intensity after a pause of 0.5s. The polariser was aligned with the LC front-face director by removing the analyser and finding the orientation producing minimum transmission. To set the position of the analyser the LC cell was removed and the analyser oriented to give either maximum or minimum transmission.

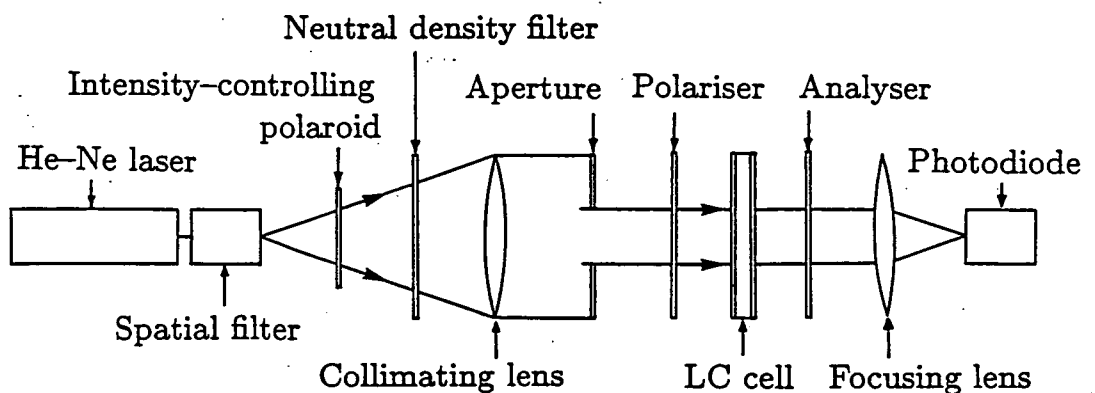


Figure 2.9: LC cell optical test bench.

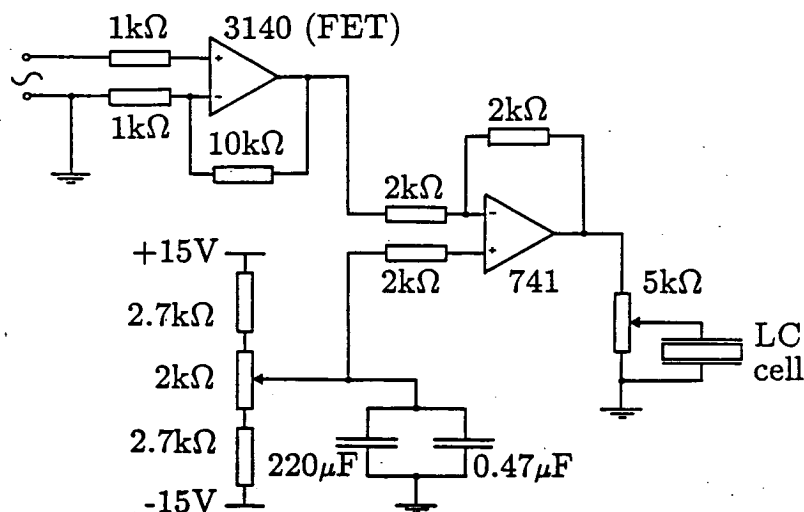


Figure 2.10: LC cell voltage control circuit.

2.7 Comparison of Theory and Experiment

Results are presented here for the experimentally measured transmission of a guest-host LC $13\mu\text{m}$ thick. These results are compared with the theoretical predictions of the model described above, with and without the molecular disorder correction. The transmittances are plotted in figure 2.11(a) and (b) for parallel and perpendicular polaroids.

In the corrected model the disorder factor, σ , was set to 2.0. The maximum iterative uncertainty is denoted by the vertical error bars. The relative scale factor for each pair of theoretical transmission curves (with and without the disorder correction) was chosen by eye to give the best overall fit to the experimental data over the range of voltages measured.

The overall correlation between theory and experiment is significantly improved when the molecular disorder correction is included. At larger voltages there is a small systematic error in the prediction of the corrected model. This is thought to arise principally because of the assumption that the magnitude of the

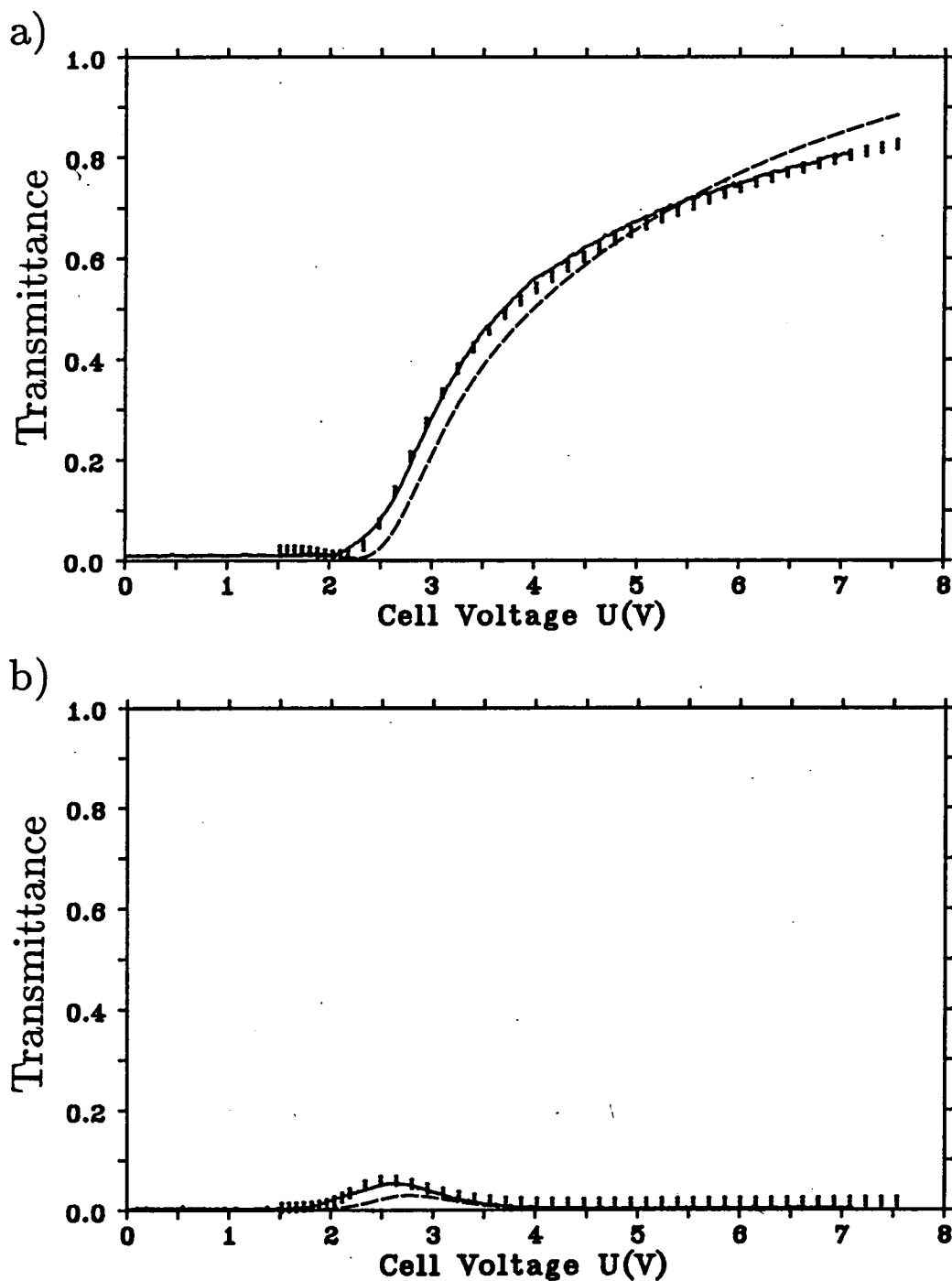


Figure 2.11: LC cell transmittance through parallel (a) and perpendicular (b) polaroids. In both cases the incident light was polarised parallel to the front-face director. The continuous curve is the experimental data, the dashed curve the uncorrected model and the points with error bars the model including the molecular disorder correction.

director orientational fluctuations is unaffected by the electric field. In practice increasing the applied field reduces the amplitude of these fluctuations so we might expect the uncorrected model to become more realistic. This would mean that in figure 2.11 the corrected theoretical curves would be closer than they are to the uncorrected curves at large fields. Then the corrected curves would match the experimental data better.

2.8 Appendix A: The Director Configuration

In this appendix the method used to calculate the nematic director configuration is presented. Montgomery[22] showed that the tilt and twist angles, θ and ϕ , are related to the position in the LC layer by the relations:

$$\frac{z}{L} = \frac{\int_0^\xi \frac{(1 + \kappa \sin^2 \theta_m \sin^2 \xi) d\xi}{(1 - \sin^2 \theta_m \sin^2 \xi)^{\frac{1}{2}} R(\theta_m, \xi)}}{\int_0^{\pi/2} \frac{(1 + \kappa \sin^2 \theta_m \sin^2 \xi) d\xi}{(1 - \sin^2 \theta_m \sin^2 \xi)^{\frac{1}{2}} R(\theta_m, \xi)}}, \quad (2.19)$$

$$\phi = \beta \int_0^\xi \frac{(1 + \kappa \sin^2 \theta_m \sin^2 \xi) d\xi}{(1 - \sin^2 \theta_m \sin^2 \xi)^{\frac{3}{2}} (1 + \alpha \sin^2 \theta_m \sin^2 \xi) R(\theta_m, \xi)} \quad (2.20)$$

where the variable ξ is defined by

$$\sin \xi = \sin \theta / \sin \theta_m, \quad (2.21)$$

β is a constant of integration and θ_m is the maximum tilt angle i.e. the tilt angle in the middle of the LC layer. In equations 2.19 and 2.20

$$\kappa = (k_{33} - k_{11})/k_{11}, \quad (2.22)$$

$$\alpha = (k_{33} - k_{22})/k_{22}, \quad (2.23)$$

$$\gamma = \Delta\epsilon/\epsilon_\perp, \quad (2.24)$$

$$R^2(\theta_m, \xi) = \frac{1}{(1 + \gamma \sin^2 \theta_m)(1 + \gamma \sin^2 \theta_m \sin^2 \xi)} + \beta^2 \left(\frac{1 + \kappa}{1 + \alpha} \right) \cdot \frac{[1 - \alpha(\cos^2 \theta_m - \sin^2 \theta_m \sin^2 \xi)]}{(1 + \alpha \sin^2 \theta_m)(1 + \alpha \sin^2 \theta_m \sin^2 \xi)(1 - \sin^2 \theta_m)(1 - \sin^2 \theta_m \sin^2 \xi)}. \quad (2.25)$$

The values of the constants θ_m and β are evaluated by solving the following coupled equations:

$$\frac{\pi}{2} = 2\beta \int_0^{\pi/2} \frac{(1 + \kappa \sin^2 \theta_m \sin^2 \xi)^{\frac{1}{2}} d\xi}{(1 - \sin^2 \theta_m \sin^2 \xi)^{\frac{1}{2}} (1 + \alpha \sin^2 \theta_m \sin^2 \xi) R(\theta_m, \xi)}, \quad (2.26)$$

$$\frac{U}{U_o} = \frac{2}{\pi} \int_0^{\pi/2} \frac{(1 + \kappa \sin^2 \theta_m \sin^2 \xi)^{\frac{1}{2}} d\xi}{(1 - \sin^2 \theta_m \sin^2 \xi)^{\frac{1}{2}} (1 + \gamma \sin^2 \theta_m \sin^2 \xi) R(\theta_m, \xi)}. \quad (2.27)$$

In these expressions U is the voltage applied across the LC and U_o is a constant defined by

$$U_o = \pi(k_{11}/\epsilon_o \Delta \epsilon)^{\frac{1}{2}}. \quad (2.28)$$

The threshold voltage U_T , below which no distortion of the director orientation occurs, is shown by Montgomery [22] to be related to U_o by

$$U_T = U_o \left[1 + \left(\frac{k_{33} - 2k_{22}}{4k_{11}} \right) \right]^{\frac{1}{2}}. \quad (2.29)$$

We found that an effective way of calculating values of θ_m and β from equations 2.26 and 2.27 for a particular voltage was to use the midpoint rule [26, p221]. The midpoint rule was then used on equation 2.19 to calculate the tilt angle at equally spaced intervals through the LC. Finally the twist angle was calculated from equation 2.20. This method proved satisfactory for $U \leq 3U_o$. However as U increases further θ_m tends rapidly towards $\pi/2$ at which point there is an infinite singularity in the integrand of equation 2.26 at the upper limit of integration. The singularity makes it more and more difficult to calculate θ_m and β accurately as the voltage increases. Welford and Sambles [20] have found an elegant solution to a similar problem which occurs in calculating the director orientation of untwisted nematics. They used the following substitutions:

$$Y = \tan^2 \theta_m, \quad (2.30)$$

$$W = \tan^2 \xi. \quad (2.31)$$

These substitutions control the singularity because $Y \rightarrow \infty$ as $\theta_m \rightarrow \pi/2$. If we employ the same substitutions in the calculation of twisted nematic director

orientations then equations 2.19, 2.20, 2.26, 2.26 and 2.27 become

$$\frac{z}{L} = \frac{1}{2} \frac{\int_0^W \frac{[(1+Y)(1+W) + \kappa WY]^{\frac{1}{2}} dW}{[W(1+Y+W)]^{\frac{1}{2}} (1+W) R(Y, W)}}{\int_0^\infty \frac{[(1+Y)(1+W) + \kappa WY]^{\frac{1}{2}} dW}{[W(1+Y+W)]^{\frac{1}{2}} (1+W) R(Y, W)}}, \quad (2.32)$$

$$\phi = \frac{\beta}{2} \int_0^W \frac{[(1+Y)(1+W) + \kappa WY]^{\frac{1}{2}} (1+Y)^2 (1+W) dW}{W^{\frac{1}{2}} (1+Y+W)^{\frac{3}{2}} [(1+Y)(1+W) + \alpha WY] R(Y, W)}, \quad (2.33)$$

$$R^2(Y, W) = (1+Y)^2 (1+W) \left\{ \frac{1}{(1+Y + \gamma Y)[(1+Y)(1+W) + \gamma WY]} + \beta^2 \left(\frac{1+\kappa}{1+\alpha} \right) \frac{(1+Y)[(1+Y - \alpha)(1+W) + \alpha WY]}{(1+Y + \alpha Y)[(1+Y)(1+W) + \alpha WY](1+Y+W)} \right\}, \quad (2.34)$$

$$\frac{\pi}{2} = \beta \int_0^\infty \frac{[(1+Y)(1+W) + \kappa WY]^{\frac{1}{2}} (1+Y)^2 (1+W) dW}{W^{\frac{1}{2}} (1+Y+W)^{\frac{3}{2}} [(1+Y)(1+W) + \alpha WY] R(Y, W)}, \quad (2.35)$$

$$\frac{U}{U_o} = \frac{1}{\pi} \int_0^\infty \frac{[(1+Y)(1+W) + \kappa WY]^{\frac{1}{2}} (1+Y) dW}{[W(1+Y+W)]^{\frac{1}{2}} [(1+Y)(1+W) + \gamma WY] R(Y, W)}. \quad (2.36)$$

Equations 2.32 to 2.36 were found to be accurately soluble for much larger voltages than the equivalent equations without the substitutions. In particular accurate solutions were obtained for voltages up to $5U_o$ which was sufficient for comparison with the experimental measurements described in section 2.6.

2.9 Appendix B: The Optical Properties

In this appendix the method which was used to calculate the optical properties of a LC cell is described. Let an electromagnetic wave travelling in the $+z$ direction (cf figure 2.5) be normally incident on the LC cell. Montgomery [16] has shown that if the total transverse electric and magnetic field components at a point within the LC are E_x , E_y , H_x and H_y , then Maxwell's equations can be written as

$$\frac{\partial \Psi}{\partial z} = \frac{i\omega}{c} \Delta \Psi \quad (2.37)$$

where Ψ is the vector

$$\Psi = [E_x, (\mu_o/\epsilon_o)^{\frac{1}{2}} H_y, E_y, -(\mu_o/\epsilon_o)^{\frac{1}{2}} H_x]^T. \quad (2.38)$$

In terms of the LC refractive indices and the director tilt and twist angles the non-zero terms of the Δ matrix are

$$\Delta_{12} = \Delta_{34} = 1, \quad (2.39)$$

$$\Delta_{21} = n_o^2(1 + \gamma \sin^2 \theta + \gamma \cos^2 \theta \cos^2 \phi)/(1 + \gamma \sin^2 \theta), \quad (2.40)$$

$$\Delta_{23} = \Delta_{41} = n_o^2 \gamma \cos^2 \theta \cos \phi \sin \phi/(1 + \gamma \sin^2 \theta), \quad (2.41)$$

$$\Delta_{43} = n_o^2(1 + \gamma \sin^2 \theta + \gamma \cos^2 \theta \sin^2 \phi)/(1 + \gamma \sin^2 \theta), \quad (2.42)$$

where

$$\gamma = (n_e^2 - n_o^2)/n_o^2. \quad (2.43)$$

If the field vector Ψ is known in the plane $z = z_o$ then, if Δ is independent of z over the interval from z_o to $z_o + h$, it can be shown that [16]

$$\Psi(z_o + h) = P(z_o, h)\Psi(z_o) \quad (2.44)$$

where

$$P(z_o, h) = I + \left(\frac{i\omega h}{c}\right) \Delta + \frac{1}{2!} \left(\frac{i\omega h}{c}\right)^2 \Delta^2 + \dots \quad (2.45)$$

In equation 2.45 I is the 4×4 identity matrix. $P(z_o, h)$ is described as the propagation matrix for the interval. We can then calculate the field vector in the plane $z_o + 2h$ by computing the propagation matrix $P(z_o + h, h)$:

$$\begin{aligned} \Psi(z_o + 2h) &= P(z_o + h, h) \Psi(z_o + h) \\ &= P(z_o + h, h) P(z_o, h) \Psi(z_o). \end{aligned} \quad (2.46)$$

Suppose that the LC layer is confined between the planes $z = 0$ and $z = L$. If the layer is divided up into slices sufficiently thin that the optical properties vary by a negligible amount across each slice i.e. equations 2.44 and 2.45 apply, then the propagation matrix for the complete LC layer is given by the product of the propagation matrices of the individual slices. If the LC layer is divided up into N slices then

$$\begin{aligned} \Psi(L) &= P((N-1)h, h), P((N-2)h, h) \dots P(h, h) P(0, h) \Psi(0) \\ &= P_{LC} \Psi(0). \end{aligned} \quad (2.47)$$

The matrix P_{LC} is the propagation matrix for the complete LC layer. P_{LC} was found by setting $N = 1000$ and truncating the expression for the slice propagation matrix (equation 2.45) after the term in Δ^5 . The most time consuming part of the whole optical calculation is the repeated multiplying out of this expression. Two methods of speeding up the calculation were considered: first the use of a closed form of the slice propagation matrix [32] and second multiplying out expression 2.45 by hand up to and including the term in Δ^5 . The former increased the speed of calculation by a factor of ten and the latter increased the speed by a factor of forty. Therefore the latter method, which exploits the sparsity of Δ and its multiples, was used throughout the work described in this thesis.

To describe the optical properties of guest host LCs it is necessary to extend the above method to take account of the absorption caused by the dichroic dye. This was done by replacing the refractive indices n_e and n_o in the Δ matrix by

$$n_e^* = n_e(1 + i\kappa_e), \quad (2.48)$$

$$n_o^* = n_o(1 + i\kappa_o). \quad (2.49)$$

The meaning of the imaginary component of a refractive index can be understood by considering a plane wave $\mathbf{E}$ propagating through a medium of refractive index $n^* = n(1 + i\kappa)$:

$$\begin{aligned} \mathbf{E} &= \mathbf{E}_0 \exp[i\omega(n^*z/c - t)] \\ &= \mathbf{E}_0 \exp(-\omega n\kappa z/c) \exp[i\omega(nz/c - t)]. \end{aligned} \quad (2.50)$$

Equation 2.50 shows that the imaginary component of a refractive index is directly proportional to the amplitude absorption coefficient $\omega n\kappa/c$. The intensity absorption coefficient is found, by taking the squared modulus of $\mathbf{E}$, to be twice the amplitude absorption coefficient. The values of κ_e and κ_o are calculated from the intensity absorption coefficients given in table 2.4.

Montgomery [16] has shown that the propagation matrix for an isotropic layer

(such as glass, ITO or MgF_2) has a closed form. For a layer of refractive index n and thickness h the propagation matrix is

$$P(z, h) = \begin{pmatrix} \cos \nu & (i/n) \sin \nu & 0 & 0 \\ (in) \sin \nu & \cos \nu & 0 & 0 \\ 0 & 0 & \cos \nu & (i/n) \sin \nu \\ 0 & 0 & (in) \sin \nu & \cos \nu \end{pmatrix} \quad (2.51)$$

where $\nu = n\omega h/c$. To find the propagation matrix for the complete LC cell, P , the propagation matrices for each layer are multiplied together:

$$P = P_{gl} P_{ITO} P_{\text{MgF}_2} P_{LC} P_{\text{MgF}_2} P_{ITO} P_{gl}. \quad (2.52)$$

The reflected and transmitted electric fields can then be computed using the matrix P . In terms of the incident electric field components E_x and E_y the reflected and transmitted electric field components R_x , R_y , T_x and T_y are [16]

$$\begin{aligned} R_x &= r_{xx}E_x + r_{xy}E_y, \\ R_y &= r_{yx}E_x + r_{yy}E_y, \\ T_x &= (g_{11} + g_{12}r_{xx} + g_{14}r_{yx})E_x + (g_{13} + g_{12}r_{xy} + g_{14}r_{yy})E_y, \\ T_y &= (g_{31} + g_{32}r_{xx} + g_{34}r_{yx})E_x + (g_{33} + g_{32}r_{xy} + g_{34}r_{yy})E_y \end{aligned}$$

where

$$\begin{aligned} r_{xx} &= [(g_{21} - g_{11})(g_{34} - g_{44}) - (g_{41} - g_{31})(g_{14} - g_{24})]/Q, \\ r_{xy} &= [(g_{23} - g_{13})(g_{34} - g_{44}) - (g_{43} - g_{33})(g_{14} - g_{24})]/Q, \\ r_{yx} &= [(g_{12} - g_{22})(g_{41} - g_{31}) - (g_{32} - g_{42})(g_{21} - g_{11})]/Q, \\ r_{yy} &= [(g_{12} - g_{22})(g_{43} - g_{33}) - (g_{32} - g_{42})(g_{23} - g_{13})]/Q, \\ Q &= [(g_{12} - g_{22})(g_{34} - g_{44}) - (g_{32} - g_{42})(g_{14} - g_{24})] \end{aligned}$$

where

$$\begin{aligned} g_{11} &= P_{11} + nP_{12}, \\ g_{12} &= P_{11} - nP_{12}, \end{aligned}$$

$$\begin{aligned}
g_{13} &= P_{13} + nP_{14}, \\
g_{14} &= P_{13} - nP_{14}, \\
g_{21} &= (P_{21} + nP_{22})/n, \\
g_{22} &= (P_{21} - nP_{22})/n, \\
g_{23} &= (P_{23} + nP_{24})/n, \\
g_{24} &= (P_{23} - nP_{24})/n, \\
g_{31} &= P_{31} + nP_{32}, \\
g_{32} &= P_{31} - nP_{32}, \\
g_{33} &= P_{33} + nP_{34}, \\
g_{34} &= P_{33} - nP_{34}, \\
g_{41} &= (P_{41} + nP_{42})/n, \\
g_{42} &= (P_{41} - nP_{42})/n, \\
g_{43} &= (P_{43} + nP_{44})/n, \\
g_{44} &= (P_{43} - nP_{44})/n,
\end{aligned}$$

where n is the refractive index of the medium surrounding the LC cell.

Chapter 3

A Method for Computing Homogeneous–Liquid–Crystal Conoscopic Figures

3.1 Measurement of LC Tilt Angles

The surface tilt angle of the director in both nematic and smectic LC devices strongly influences the device performance. In twisted nematic LC cells, with a total twist angle of 90° , a small but non-zero surface tilt angle prevents regions of opposite tilt angle forming when a voltage is applied thus avoiding light scattering at the interfaces between these regions. However too large a tilt angle reduces the contrast ratio and multiplexability of the device and increases the viewing-angle dependent colouration [33,34]. In supertwisted nematic LC cells, with a total twist angle of 270° , a large (typically $20 - 30^\circ$) surface tilt angle is required to stabilise the highly distorted director configuration [35,36]. The bistable electro-optic effect in SmC^* LCs is based on the surface-stabilisation of the director configuration and requires a zero or small surface tilt angle [37]. Uniform surface director alignment and tilt angle are essential in each of the above cases. The methods most commonly used to produce small or zero sur-

face tilt angles are described in section 2.1 and a more general discussion of alignment techniques is given in the review article by Cognard [38]. If the two surfaces of the LC cell are treated so as to produce a uniformly tilted director orientation throughout the LC then the tilt angle can be measured by one of the following methods.

Conoscopy. Information about the director orientation may be obtained by examining the sample with a polarising microscope in convergent light between crossed polarisers. The pattern of interference fringes and extinction positions that is produced in the back focal plane of the microscope objective lens is characteristic of the LC birefringence and director orientation with respect to the microscope axis. A number of techniques can be used to determine the director tilt angle [34] but if the tilt angle is small, as it is in all the LC cells considered here, then only one of them is applicable. A universal stage [39, p396ff] is fitted to the microscope and is used to orientate the LC cell so that the uniaxial flash figure (see section 3.4.2) is obtained. The director tilt angle may then be calculated by reading the cell tilt angle from the universal stage scale and correcting for refraction at the LC surfaces. However, accurate measurement is difficult, because of the diffuseness of the uniaxial flash figure, and tedious because of the difficulty of mounting the sample on a universal stage.

Capacitance Measurement. Measurement of the capacitance of a LC layer can provide a measurement of the director tilt angle [33]. The zero-field capacitance C of a cell filled with LC of constant director orientation is given by

$$C = C_o(\epsilon_{\parallel} \sin^2 \theta + \epsilon_{\perp} \cos^2 \theta) \quad (3.1)$$

where C_o is the empty cell capacitance, $\epsilon_{\parallel}$ and $\epsilon_{\perp}$ are the dielectric constants parallel and perpendicular to the director and θ is the director tilt angle. θ may be calculated by rearranging equation 3.1. However, the accuracy of the result depends upon the accuracy of the other measurements.

Also, care must be taken that the voltage used to measure the capacitance does not measurably distort the uniform director configuration [33]. Finally the technique is not applicable in this form to SmC* LCs because they are biaxial at the frequencies used to measure the LC capacitance.

Magnetic Null Method. In this technique the LC cell is rotated in a uniform magnetic field until the orientation is found where a measured physical property, such as the optical retardation, is independent of the magnetic field strength [33]. At this null orientation the director tilt angle is identical to the angle between the magnetic field lines and the cell orientation. This technique is accurate to within a fraction of one degree and is applicable to any tilt angle.

In this chapter a technique is presented which overcomes the principal limitations of the conoscopic technique and allows small director tilt angles to be measured to within an accuracy of one degree while avoiding the need for a universal stage. Although the technique presented is slightly less accurate than the magnetic null method it is much simpler to perform.

Figure 3.1 is a schematic diagram showing a polarising microscope set up for conoscopic observation. A parallel beam of light is passed in sequence through a polariser, a condenser lens system, an optically anisotropic sample, an objective lens system and an analyser which is crossed with respect to the polariser. The conoscopic figure is the interference pattern formed by the ordinary and extraordinary waves in the back focal plane of the objective lens system [40, chapter 9]. In a polarising microscope this plane is before the analyser. The Bertrand lens is inserted so that the figure may be viewed through the analyser with the ocular lens system. When observed in white light the figure is composed of lines of equal colour (isochromes) and extinction positions (isogyres). If monochromatic light illuminates the sample then the isochromes constitute a pattern of dark and light fringes instead. Both isochromes and isogyres yield information about

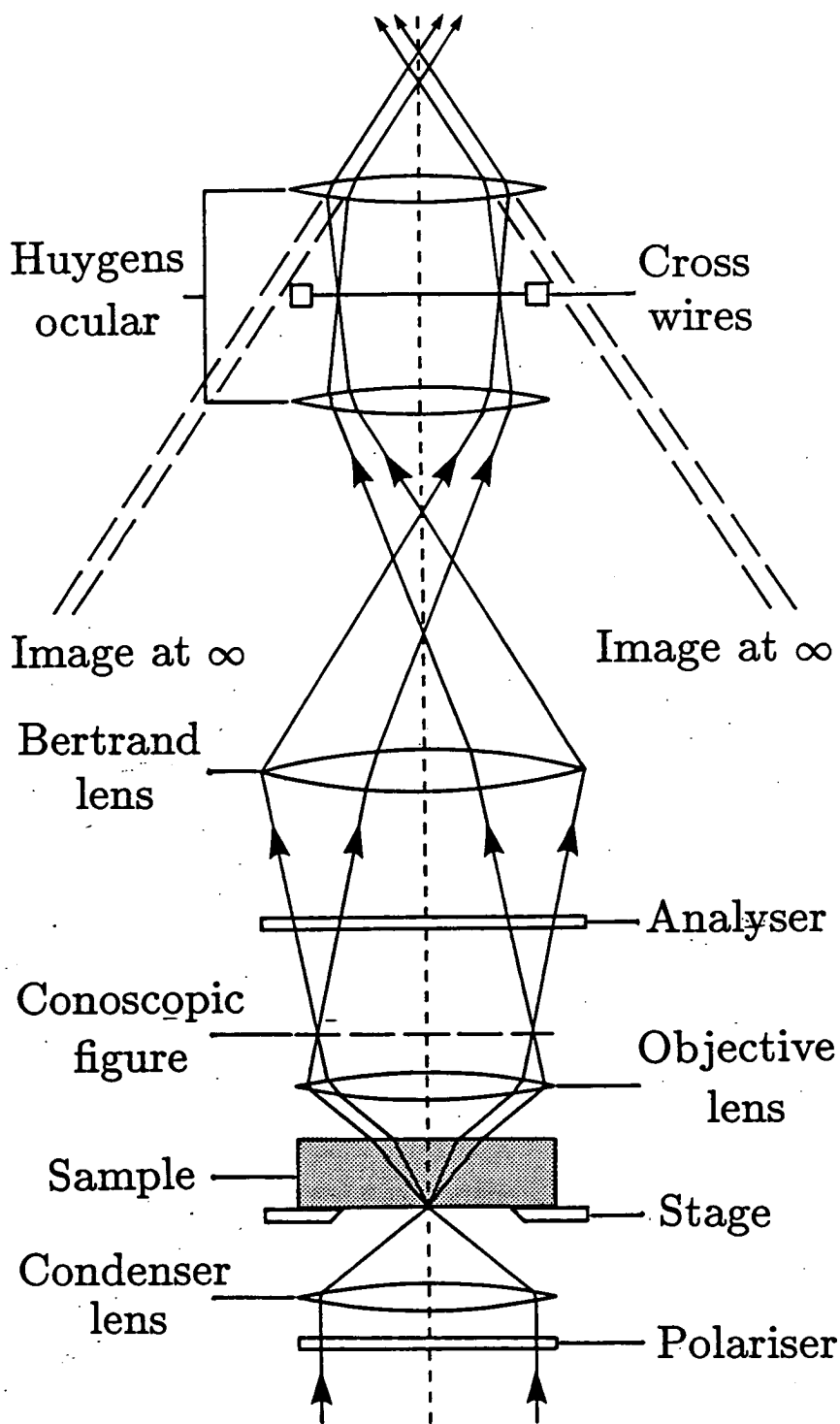


Figure 3.1: Schematic diagram of a polarising microscope. The wavefront incident on the optically anisotropic sample is split into ordinary and extraordinary components. The conoscopic figure is the interference pattern formed by the transmitted light in the back focal plane of the objective lens. An image of the figure at infinity is produced by the Bertrand lens and the ocular.

the orientation of the optic axis/axes. In particular, for a uniaxial sample the pattern of isochromes and isogyres, and the way in which this pattern moves when the sample is rotated, provides information about the angle at which the optic axis is tilted out of the plane of section.

In this chapter a method is presented for computing the conoscopic figures produced by complete LC cells with uniform director orientation throughout the LC thickness. The calculated figures are interpreted in terms of Bertin's surfaces (surfaces of constant phase difference between the ordinary and extraordinary waves) and the influence of the Fresnel coefficients on the figures is shown. Examples of calculated conoscopic figures are presented including the symmetric flash figure (zero tilt) and the optic-normal figure (90° tilt). The way in which these characteristic figures are altered by small orientational changes of the director is demonstrated. A model of the microscope condenser and objective lens systems is introduced to enable computation of the lens-induced polarisation. This effect is then incorporated into the conoscopic calculations and the effect on the figures is shown. A set of calculated conoscopic figures is produced for different director tilt angles. Finally the experimental conoscopic figure for a $7\mu\text{m}$ thick chiral smectic C (SmC^*) LC is compared with the calculated figures and the director-tilt angle is determined.

3.2 Optical Description of a Homogeneous LC Cell

3.2.1 Light Propagation in a Uniaxial Medium

A variety of methods has been developed previously to investigate the propagation of light in a uniaxial layered medium [42,43] or [44, chapter 9.7]. These

methods provide an exact solution to the problem and take account of refraction and multiple reflections between interfaces. However in the method described below multiple reflections were neglected as they usually have only a small effect on the transmitted electric field. This simplified treatment, based on that of Yeh [44, chapter 9.5–6], was found sufficient to describe all the experimentally observed phenomena associated with conoscopic figures and is much faster computationally than the exact methods. In this chapter Yeh's method is extended to allow any orientation of the director and to take account of isotropic layers on either side of the LC layer. A previous method of calculating LC conoscopic figures [45] was considered unsuitable because it ignores all reflections at interfaces.

Consider a uniaxial plate of thickness d and refractive indices n_e and n_o positioned as shown in figure 3.2a. As shown in figure 3.2b the angles θ and ϕ define the tilt and twist of the director, $\mathbf{n}$. A plane wave with angular frequency ω and wave vector $\mathbf{K}$ is incident at angle χ , in the yz plane, on the front surface of the plate. At this surface the wave is divided into a reflected component, with wave vector $\mathbf{K}'$, and two transmitted components, the ordinary and extraordinary, with wave vectors $\mathbf{K}_o$ and $\mathbf{K}_e$. At the second surface the ordinary and extraordinary waves are reflected, with wave vectors $\mathbf{K}'_o$ and $\mathbf{K}'_e$, and transmitted, with wave vector $\mathbf{K}$.

At the first surface the incident, reflected and transmitted electric field vectors are

$$\mathbf{E}_i(z=0) = (A_s \hat{\mathbf{s}} + A_p \hat{\mathbf{p}}) \exp[i\omega t], \quad (3.2)$$

$$\mathbf{E}_r(z=0) = (B_s \hat{\mathbf{s}} + B_p \hat{\mathbf{p}}') \exp[i\omega t], \quad (3.3)$$

$$\mathbf{E}_t(z=0) = (C_o \hat{\mathbf{o}} + C_e \hat{\mathbf{e}}) \exp[i\omega t], \quad (3.4)$$

where $\hat{\mathbf{s}}$ is a unit vector perpendicular to the plane of incidence and is given by $\hat{\mathbf{s}} = \mathbf{x}$ as shown in figure 3.2a. $\hat{\mathbf{p}}$ and $\hat{\mathbf{p}}'$ are unit vectors parallel to the plane

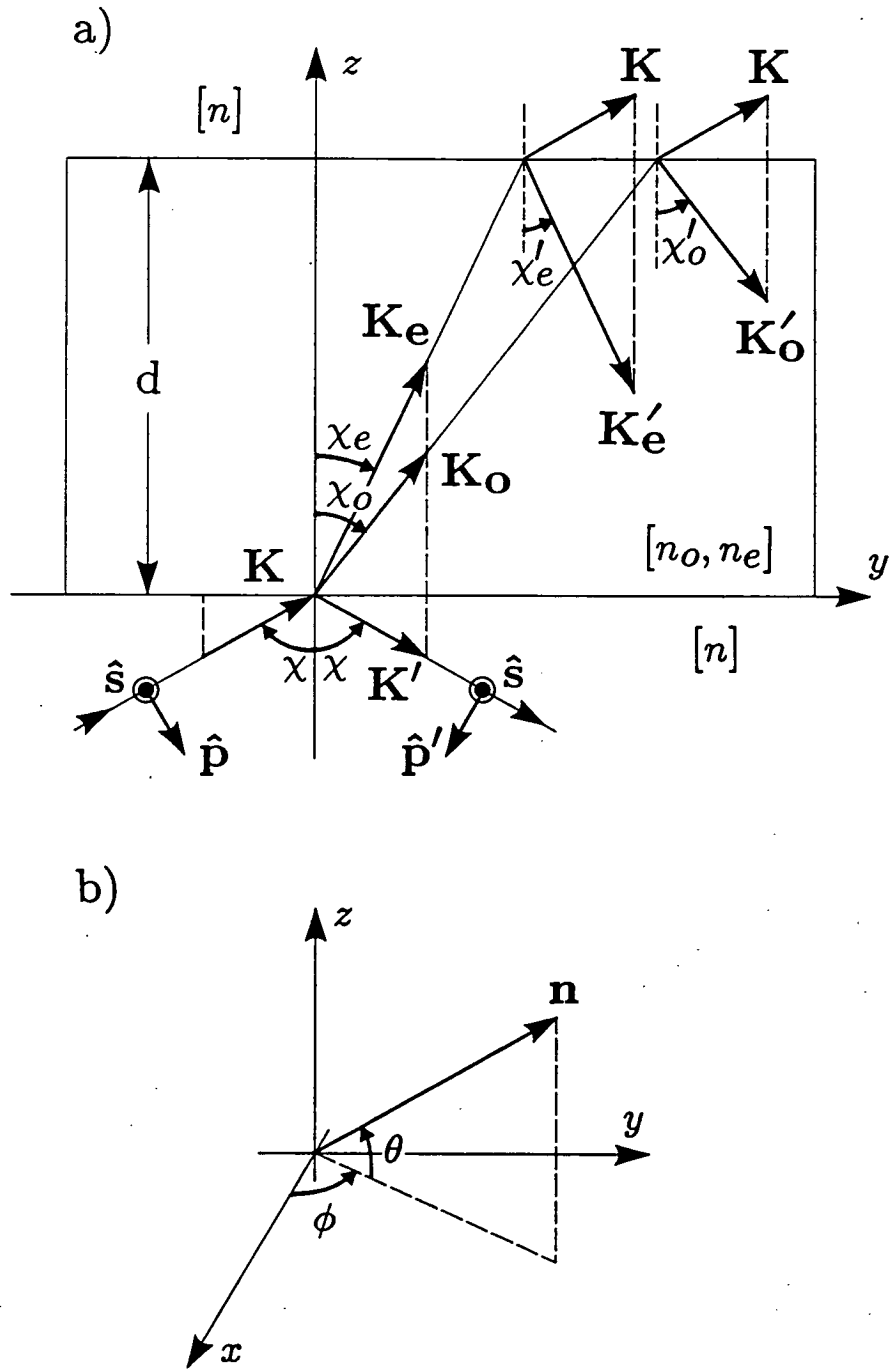


Figure 3.2: a) Reflection and refraction of light incident on a uniaxial slab within an isotropic medium. The wave vectors of the incident, reflected, forward-propagating ordinary and extraordinary and backward-propagating ordinary and extraordinary waves are $\mathbf{K}$, $\mathbf{K}'$, $\mathbf{K}_o$, $\mathbf{K}_e$, $\mathbf{K}'_o$ and $\mathbf{K}'_e$ respectively. $\hat{\mathbf{s}}$ is a unit vector perpendicular to the plane of incidence and $\hat{\mathbf{p}}$ and $\hat{\mathbf{p}}'$ are unit vectors parallel to the plane of incidence. b) Definition of the tilt (θ) and twist (ϕ) angles of the nematic director $\mathbf{n}$.



of incidence and are given by

$$\hat{\mathbf{p}} = \mathbf{K} \times \hat{\mathbf{s}} / |\mathbf{K}|, \quad (3.5)$$

$$\hat{\mathbf{p}}' = \mathbf{K}' \times \hat{\mathbf{s}} / |\mathbf{K}'|. \quad (3.6)$$

$\hat{\mathbf{o}}$ and $\hat{\mathbf{e}}$ are unit vectors parallel to the electric field vectors of the ordinary and extraordinary waves in the uniaxial medium.

At the first surface the tangential components of the wave vectors, β , are equal so we may write

$$\mathbf{K} = \beta \mathbf{y} + K_z \mathbf{z}, \quad (3.7)$$

$$\mathbf{K}' = \beta \mathbf{y} - K_z \mathbf{z}, \quad (3.8)$$

$$\mathbf{K}_o = \beta \mathbf{y} + K_{oz} \mathbf{z}, \quad (3.9)$$

$$\mathbf{K}_e = \beta \mathbf{y} + K_{ez} \mathbf{z}. \quad (3.10)$$

Let n be the refractive index of the surrounding medium so that

$$\beta = (\omega/c)n \sin \chi \quad (3.11)$$

and K_z , the z -component of $\mathbf{K}$, is given by

$$K_z = (\omega/c)n \cos \chi. \quad (3.12)$$

Expressions for the z -components of $\mathbf{K}_o$ and $\mathbf{K}_e$, K_{oz} and K_{ez} , are given in appendix A. The ordinary and extraordinary refraction angles, χ_o and χ_e , are found using equations 3.9 and 3.10:

$$\chi_o = \arctan(\beta/K_{oz}), \quad (3.13)$$

$$\chi_e = \arctan(\beta/K_{ez}). \quad (3.14)$$

The ordinary and extraordinary refractive indices are n_o and $n_e(\chi_e)$ where

$$n_e(\chi_e) = \frac{K_{ez}}{(\omega/c) \cos \chi_e}. \quad (3.15)$$

The unit vectors $\hat{o}$ and $\hat{e}$ are (appendix B):

$$\hat{o} = N_o \mathcal{M}(-\beta \cos \phi, \beta \sin \theta \sin \phi - K_{oz} \cos \theta, 0)^T, \quad (3.16)$$

$$\hat{e} = N_e \mathcal{M} \left(\frac{K_{ez} \cos \theta - \beta \sin \theta \sin \phi}{n_e^2(\chi_e) - n_o^2}, \frac{-\beta \cos \phi}{n_e^2(\chi_e) - n_o^2}, \frac{K_{ez} \sin \theta + \beta \cos \theta \sin \phi}{n_e^2(\chi_e) - n_e^2} \right)^T, \quad (3.17)$$

where N_o and N_e are normalising constants, $\mathcal{M}$ is the rotation matrix given in appendix A relating the components of a vector in the dielectric ellipsoid frame of reference to those in the xyz frame. Since we have defined the electric field vectors fully the magnetic field vectors can be derived from Maxwell's equations. As Yeh [44, chapter 9.6] shows, the continuity of the tangential components of the electric and magnetic field vectors leads to equations for the ordinary and extraordinary electric field amplitudes C_o and C_e . His equations 9.6 – 28 and 9.6 – 29 may be used directly by replacing his expressions for the wave vectors and field vectors by the more general expressions derived here.

At the second surface the incident, reflected and transmitted electric field vectors are

$$\mathbf{E}_i(z = d) = (C_o \hat{o} \exp[-iK_{oz}d] + C_e \hat{e} \exp[-iK_{ez}d]) \exp[i\omega t], \quad (3.18)$$

$$\mathbf{E}_r(z = d) = (C'_o \hat{o}' + C'_e \hat{e}') \exp[i\omega t], \quad (3.19)$$

$$\mathbf{E}_t(z = d) = (A'_s \hat{s} + A'_p \hat{p}) \exp[i\omega t], \quad (3.20)$$

where $\hat{o}'$ and $\hat{e}'$ are unit vectors parallel to the electric field vectors of the reflected ordinary and extraordinary waves, C'_o and C'_e are their complex amplitudes and A'_s and A'_p are the complex amplitudes of the transmitted electric field vectors. At the second surface the tangential components of the wave vectors are equal so we may write

$$\mathbf{K}'_o = \beta \mathbf{y} + K'_{oz} \mathbf{z}, \quad (3.21)$$

$$\mathbf{K}'_e = \beta \mathbf{y} + K'_{ez} \mathbf{z}. \quad (3.22)$$

Expressions for the z -components of $\mathbf{K}'_o$ and $\mathbf{K}'_e$, K'_{oz} and K'_{ez} , are given in appendix A. The refraction angles χ'_o and χ'_e , the refractive index $n_e(\chi'_e)$ and the

unit vectors $\hat{o}'$ and $\hat{e}'$ are determined from equations 3.13 to 3.17 by replacing the (unprimed) variables describing the forward-propagating waves with the (primed) variables describing the backward-propagating waves. As at the front surface, the magnetic field vectors may be written down in terms of the electric field vectors. The continuity of the tangential components of the electric and magnetic field vectors is then expressed as a set of four simultaneous equations (see reference [44] for details). These are solved for the complex amplitudes C'_o, C'_e, A'_s and A'_p . If we ignore multiple reflections then the amplitudes of the transmitted waves are simply given by A'_s and A'_p .

3.2.2 Light Propagation in an Isotropic Medium

The method described above must be augmented to take account of isotropic layers if a complete LC cell, shown schematically in figure 3.3, is to be modelled. On each side of the LC is a rubbed nylon alignment layer which produces uniform alignment of the LC molecules, a transparent conductive coating (indium tin oxide) and a layer of glass. At each interface the amplitude transmission and reflection coefficients are described by Fresnel's equations. Consider an interface between two isotropic media of refractive indices n_1 and n_2 . A plane wave is incident at angle χ_1 to the interface normal. If the electric field components parallel and perpendicular to the plane of incidence are E_p and E_s , then the transmitted components T_p and T_s are given [46, chapter 1.5] by

$$T_p = E_p \left(\frac{2n_1 \cos \chi_1}{n_2 \cos \chi_1 + n_1 \cos \chi_2} \right), \quad (3.23)$$

$$T_s = E_s \left(\frac{2n_1 \cos \chi_1}{n_1 \cos \chi_1 + n_2 \cos \chi_2} \right), \quad (3.24)$$

where χ_2 is the direction of propagation of the transmitted wave and is related to χ_1 by Snell's law. These equations are used to describe the transmission at each interface between isotropic media in the LC cell. The amplitudes A_s and A_p are modulated at each interface before the light reaches the LC layer and the

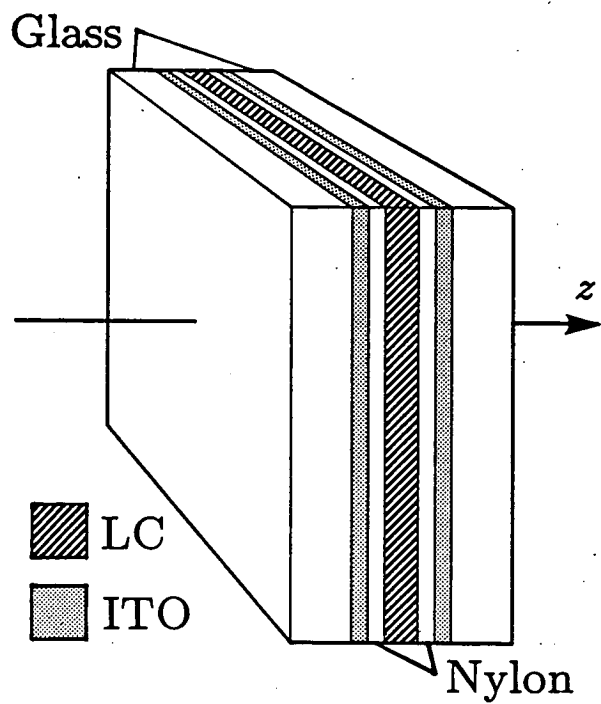


Figure 3.3: Schematic diagram of a LC cell showing the rubbed nylon alignment layers, the transparent indium tin oxide (ITO) electrodes are the glass substrates. The z -axis is parallel to the microscope axis.

amplitudes A'_s and A'_p are modulated at each interface after the LC layer.

3.3 Simulation of Conoscopic Figures

We now apply the optical method outlined in section two to the calculation of the conoscopic figures produced by a cell containing homogeneously aligned LC. It will be assumed that the polariser and (crossed) analyser are perfect polarisers for normally incident light and that the condenser and objective lens systems are free from spherical and other aberrations for the monochromatic light used. Figure 3.4 shows the coordinate systems used in the conoscopic calculations. In the simulation r_{max} is the lens radius and the radius of the field-of-view and χ_{max} is the maximum angle of incidence to the LC cell. The complete optical system is fixed in space in the $x'y'z$ coordinate system and the xyz coordinate system is related to it by the angle ρ . The x' -axis is the polariser axis and y' -axis is the analyser axis. In the $x'y'z$ system the projection of the LC director onto the $x'y'$ plane makes an angle of ϕ' with the x' axis. Therefore in the xyz system the angle ϕ is given by $\phi' - \rho$. Light passing through the polariser at point P at radius r will pass through the analyser at point Q . The angle of incidence χ is given by

$$\tan \chi = \frac{r \tan \chi_{max}}{r_{max}}. \quad (3.25)$$

If the amplitude of the electric field vector of the light transmitted by the polariser is E then, neglecting the Fresnel coefficients of the lenses as a first approximation, after passing through the lens

$$A_s = E \cos \rho, \quad (3.26)$$

$$A_p = -E \sin \rho. \quad (3.27)$$

The method of section two is then applied to calculate the complex amplitudes A'_s and A'_p transmitted by the LC cell. After passing through the objective lens

system and the analyser the complex amplitude transmittance T is given by

$$T = A'_s \sin \rho + A'_p \cos \rho \quad (3.28)$$

and the intensity transmittance is given by the squared modulus of T . The conoscopic image is built up by calculating the intensity transmittance at each point on a square grid within a circle of radius r_{maz} .

Although the lens-induced polarisation normally plays only a minor role in determining the form of the conoscopic figure (cf section 3.4.3) there are circumstances in which the effect is important. In particular, if the uniaxial medium produces a small phase difference between the ordinary and extraordinary waves the conoscopic figure may be dominated by the effect of the lenses. To take account of this possibility the Fresnel coefficients of the microscope lenses were estimated by modelling each with the lens triplet shown in figure 3.5. It was designed to be free from spherical aberration and to refract the light by a similar amount at each lens. Lens 1 in the triplet is a sphero-ellipsoid [47, chapter 5] and transforms a plane wave incident on the ellipsoidal surface into a spherical wave converging towards the second focus of the ellipsoid. Lenses 2 and 3 are aplanats [48, chapter 5] which decrease the radius of curvature of the wavefront. In each of the three lenses the radius of curvature of the back surface is matched to the wavefront curvature.

First we consider the condenser lens system shown in figure 3.5. The Fresnel coefficients for the lens when $\chi = \chi_3$ were calculated as follows. Let θ_{il} and θ_{tl} be the angles of incidence and transmission at the front surface of lens l and let χ_l be the angle which the transmitted ray makes with the z -axis. It can be shown [48, chapter 5] that for the aplanatic lens 3, $\theta_{i3} = \chi_3$ and $\theta_{t3} = \chi_2$, so that Snell's law may be written as

$$\chi_2 = \arcsin \left(\frac{n \sin \chi_3}{n_{gl}} \right), \quad (3.29)$$

where n_{gl} is the refractive index of the lens. From these relationships the Fresnel coefficients (equations 3.23 and 3.24) for the lens may be calculated. In the same

way the coefficients for lens 2 may then be calculated. At the front surface of lens 1, $\theta_{i1} = \theta_{t1} + \chi_1$. Substituting this relationship into Snell's law and rearranging we obtain

$$\theta_{t1} = \arctan \left(\frac{n \sin \chi_1}{n_{gl} - n \cos \chi_1} \right). \quad (3.30)$$

Therefore the Fresnel coefficients for lens 1 may be calculated, as may the coefficients for the complete condenser triplet, by multiplying together the coefficients for each component. The objective lens system was modelled by reversing the condenser triplet described above and calculating the Fresnel coefficients in the same way.

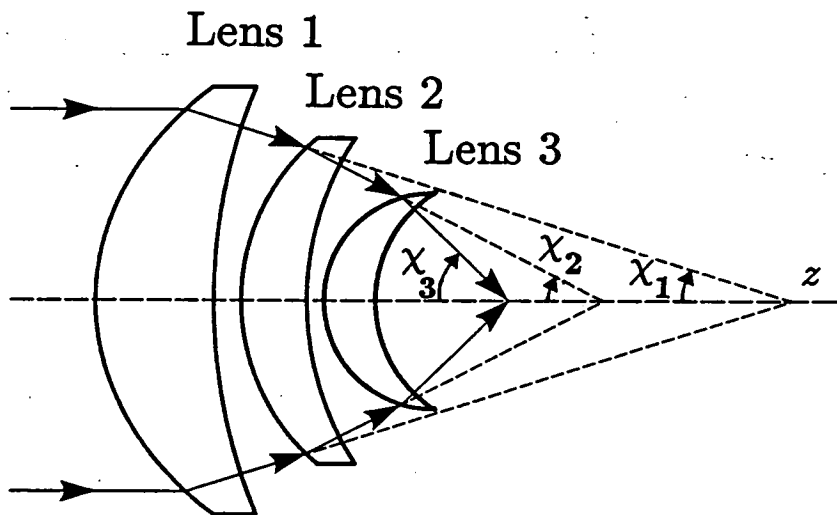


Figure 3.5: Lens triplet, consisting of a sphero-ellipsoidal (1) and two aplanatic (2 and 3) lenses, used to model the microscope condenser lens system. The same triplet was reversed to model the objective lens system.

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3.4 Interpretation of Conoscopic Figures

3.4.1 Bertin's Surfaces

As noted in section 3.1 conoscopic figures may be described in terms of two components: isochromes and isogyres. Isochromes are contour lines joining parts of the figure which have the same phase difference between ordinary and extraordinary waves. In polychromatic light isochromes appear as lines of equal colour and in monochromatic light as lines of equal fringe brightness. Isogyres are the extinction positions in the figure which correspond to optical paths for which only ordinary or only extraordinary waves are excited. When the LC cell is rotated about the z -axis the isochromes rotate with the cell whereas the isogyres either remain stationary or move relative to the isochromes in a way that depends on the director-tilt angle.

If we temporarily ignore the refraction which occurs at the LC surfaces the shape of the isochromes can be understood by considering Bertin's surfaces. Figure 3.6 shows the centre sections of Bertin's surfaces in a uniaxial medium for phase differences of one, two and three wavelengths. The surfaces indicate the distance that light must travel from the point O in any direction to produce a specified phase difference between the ordinary and extraordinary waves. Normal to the optic axis the surfaces are circular in cross-section. Within a slab of uniaxial material of thickness d the positions of the isochromes are determined (if refraction is neglected) by the intersections of Bertin's surfaces with the plane $z = d$. In general the phase difference introduced between the ordinary and extraordinary waves, Δ , is given by

$$\Delta = (K_{ex} - K_{oz})d. \quad (3.31)$$

If the phase difference is an integral number of wavelengths extinction occurs but if the phase difference is an odd number of half-wavelengths the transmittance is maximised. In fact the positions of the isochromes are altered somewhat from

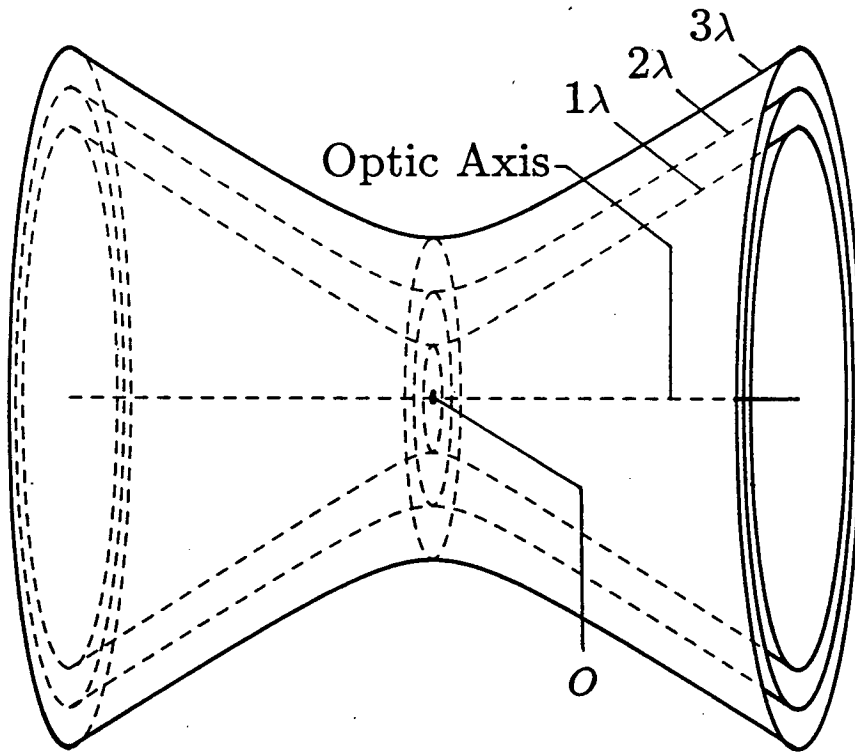


Figure 3.6: Centre section of the first three Bertin's surfaces corresponding to phase differences of one, two and three wavelengths. The surfaces connect points of equal phase difference between the ordinary and extraordinary waves emanating from the point O .

the positions described above by refraction at the LC interfaces. However the Bertin's surfaces still provide a good qualitative explanation of the form of the isochromes.

3.4.2 Characteristic Conoscopic Figures

There are certain director-orientations which give characteristic conoscopic figures. These are illustrated in the following examples where the data given in table 3.1 are used in the model of sections 3.2 and 3.3 to describe a LC cell as shown schematically in figure 3.3 but without the ITO layers. The LC refractive

Wavelength of light (sodium D-line), λ	589.3nm
LC extraordinary refractive index, n_e	1.69
LC ordinary refractive index, n_o	1.50
Nylon alignment-layer refractive index, n_{nyl}	1.53
Glass refractive index, n_{gl}	1.54

Table 3.1: Optical constants used in the conoscopic calculations

indices used are for the SmC* liquid crystal SCE3 (B.D.H. Limited). In each example the transmitted intensities were calculated for a circular field-of-view with 256 values plotted across the diameter. The contrast of the resulting image was then enhanced using histogram equalisation [49] to emphasise the form and symmetry of the pattern. Experimentally the image enhancement was carried out photographically by pushing the contrast during development and printing but could equally well have been done using an array camera, frame-grabber and histogram equalisation. So far the polarising effect of the lenses has been ignored but it will be considered in section 3.4.3.

Symmetric/Uniaxial Flash Figure

The conoscopic figures produced by rotating the sample about the z -axis when the director is in the plane of the LC cell ($\theta = 0$) are collectively called the symmetric or uniaxial flash figure [50, chapter 7] on account of the rapid appearance and disappearance of the isogyres. When the director is aligned with the polariser axis ($\phi' = 0$) the isogyres form a dark symmetric cross as shown in figure 3.7a. As the sample is rotated away from this position in either direction the cross breaks up into two hyperbolic isogyres which separate rapidly (figure 3.7b) and leave the field-of-view in the quadrants containing the optic axis. In this configuration the orientations of Bertin's surfaces are shown in figure 3.7c. Only the 2λ -surface (where λ is the wavelength of the illuminating light) intersects the LC surface within the field-of-view and it is this which causes the broadening of the vertical arms of the isogyres relative to the horizontal arms. However the isochrome is very indistinct for two reasons: refraction at the LC surface rotates the polarisation away from the director; and because the Bertin's surface crosses the LC surface at a small angle which reduces the fringe contrast. The effect of the refraction can be seen by noting the way in which the polarisation is rotated if an isotropic slab replaces the LC cell as shown in figure 3.7d. Rotation away from the x' -axis is exaggerated by a factor of four in this plot.

If the tilt angle is set at 5° , as shown in figure 3.8, the isochrome is much more easily visible and remains so as it rotates with the sample. In comparison with the symmetric flash figure the symmetry of the isogyres is clearly altered and this enables the small change in director-orientation to be detected. As the director tilt is increased the symmetric cross is further distorted and the contrast of the isochromes increases as the Bertin's surface is intersected by the LC surface at larger angles.

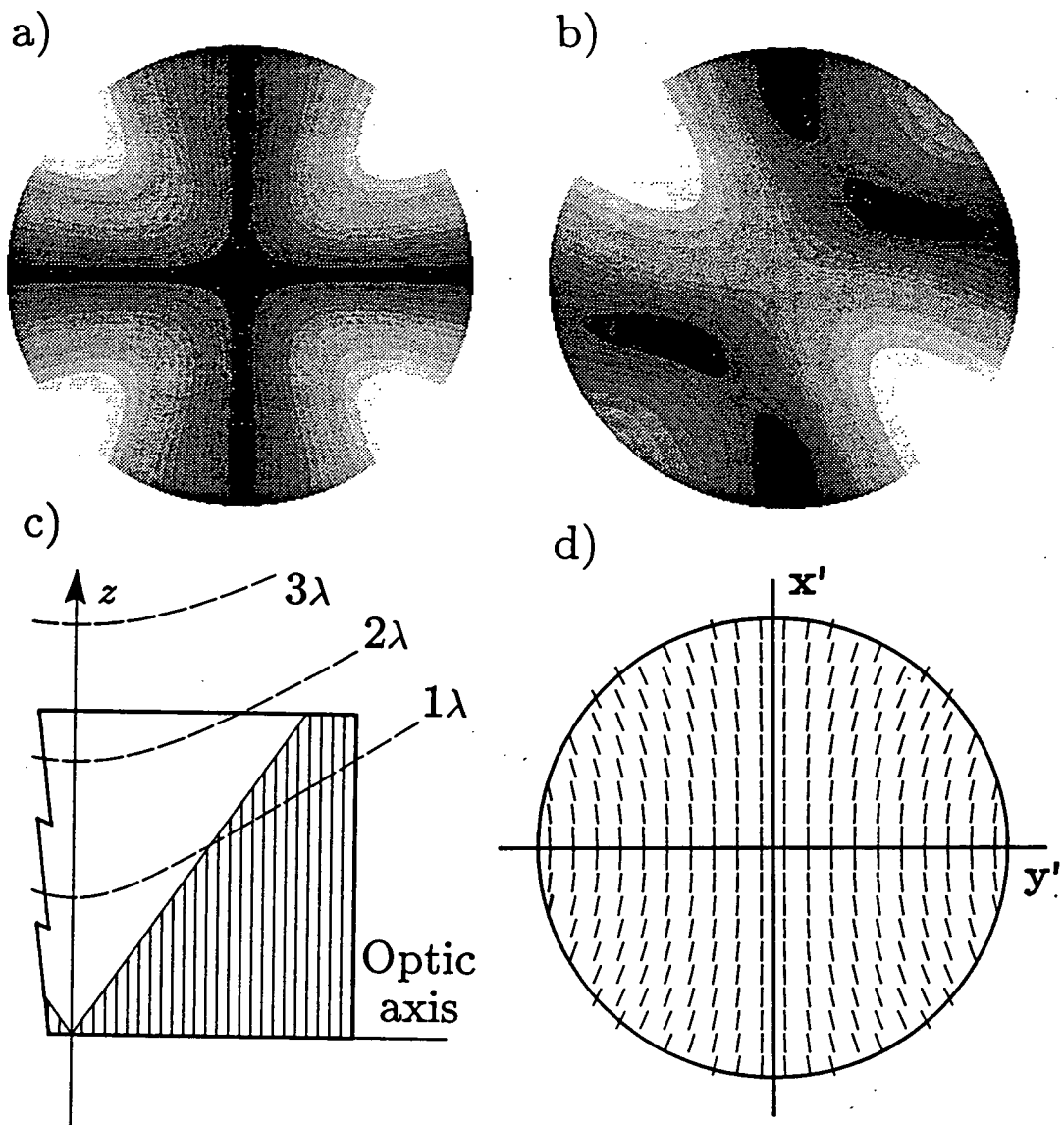


Figure 3.7: The symmetric flash figure produced by a cell containing homogeneously aligned LC with no director tilt ($\theta = 0$) and a) $\phi' = 0$ and b) $\phi' = 3^\circ$. In a) the isogyres form a dark cross which breaks up into two hyperbolic isogyres as shown in b) when the sample is rotated. c) A cross section through the LC layer showing the cone of light and the Bertin's surfaces. The intersection of the 2λ surface with the LC surface, the 2λ isochrome, causes the broadening of the vertical arms of the isogyre relative to the horizontal arms but no other part of the isochrome is visible. d) Rotation of the polarisation of light by refraction at the surfaces of an isotropic slab on the microscope stage. The polarisation rotation (away from the x' axis) has been exaggerated by a factor of four and was calculated for a slab of refractive index 1.6. It is this effect which obscures the isochrome in a) and b).

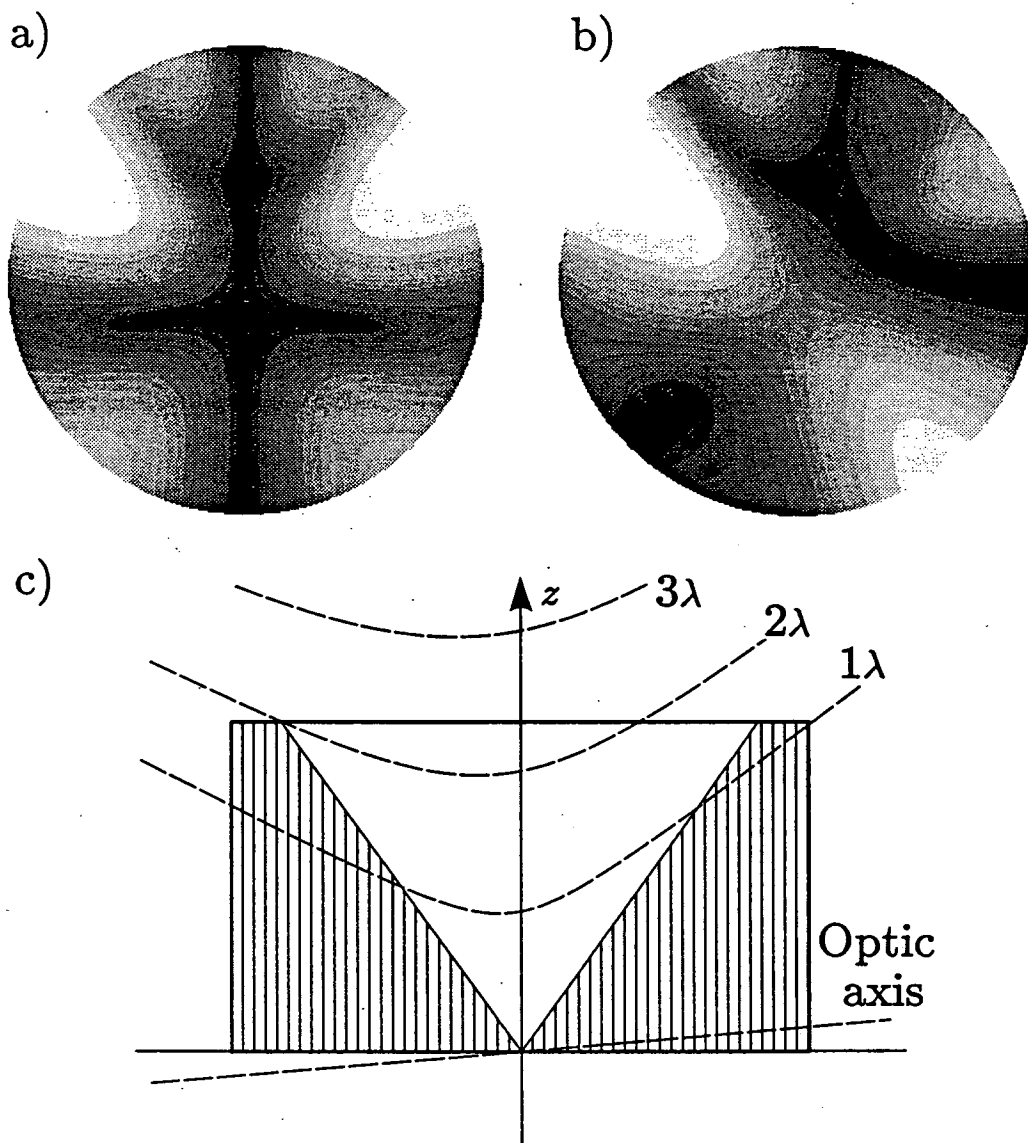


Figure 3.8: Conoscopic figures produced by a LC cell with $\theta = 5^\circ$ and a) $\phi' = 0^\circ$ and b) $\phi' = 3^\circ$. The 2λ Bertin's surface shown in c) produces the isochrome in the upper part of the figure. When the LC cell is rotated the isogyre breaks in two but the isochrome rotates unchanged with the cell.

Optic-Normal Figure

The optic-normal conoscopic figure [50, chapter 7] is produced when the director is normal to the plane of the LC ($\theta = 90^\circ$). As shown in figure 3.9a the isogyres form a dark cross centered on the optic axis which, unlike the cross of the uniaxial flash figure, remains unchanged when the sample is rotated. Figure 3.9b shows the orientation of Bertin's surfaces and the reason why no isochromes are visible. If the optic axis is tilted away from the normal position by 5° (i.e. $\theta = 85^\circ$) the cross centre follows it across the field-of-view as shown in figure 3.10a. When the LC cell is rotated the centre of the cross again follows the optic axis but the orientation of the cross remains unchanged (figure 3.10b).

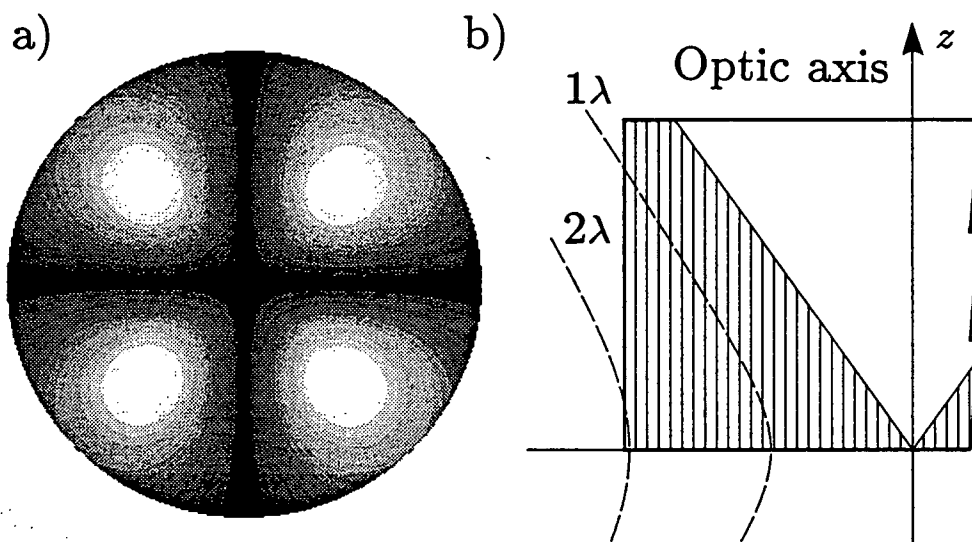


Figure 3.9: a) The optic normal ($\theta = 90^\circ$) conoscopic figure and b) the corresponding orientation of Bertin's surfaces. No isochromes are visible as none of the Bertin's surfaces intersect the LC surface within the field of view.

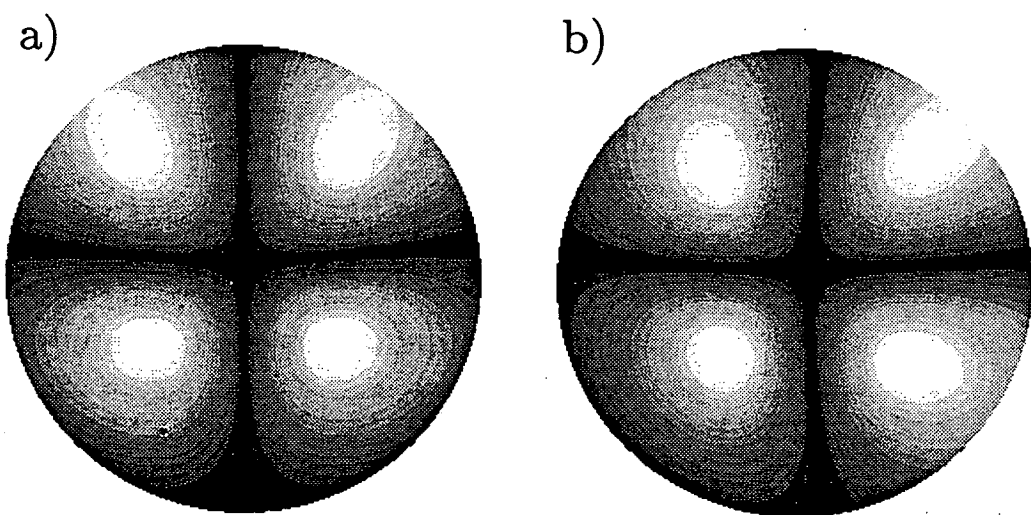


Figure 3.10: Conoscopic figures produced by a LC cell with $\theta = 85^\circ$ and a) $\phi' = 0^\circ$ and b) $\phi' = 45^\circ$. The centre of the isogyre cross lies directly over the LC optic axis in both figures and the cross retains its orientation as the LC cell is rotated.

Intermediate Figures

Conoscopic figures for tilt angles of 10° to 80° are shown in figure 3.11. As the tilt angle increases the 2λ -isochrome moves down the field of view, the 1λ -isochrome enters the field of view followed by the optic axis and finally the 2λ -isochrome leaves the foot of the field-of-view.

3.4.3 Lens-Induced Polarisation

In all of the above calculations the polarising effect of the microscope condenser and objective lenses was ignored. However the effect can be modelled, as described in section 3.3, and included in the calculation of the conoscopic figures. A refractive index of 1.519, that of the low-dispersion glass BK7, was assumed. The polarising effect of the lenses is most easily seen when the LC cell is removed altogether and the isotropic cross [51] is formed. It is shown in figure 3.12 along with a plot showing the polarisation-rotation produced by a pair of the triplet lenses described in section 3.3. In the polarisation plot each line represents the polarisation direction after passing through the lenses. The deviation from the vertical has been exaggerated by a factor of four for the sake of clarity. Figures 3.12c and d show two conoscopic figures calculated when the lens-induced polarisation was taken into account. Most obvious is the effect on the isochrome which is completely eliminated in figure 3.12c. By contrast the isogyre positions are largely maintained though their shape is altered. The alteration in the figures caused by the lens-induced polarisation is concluded to be of importance if quantitative measurements are to be made on real conoscopic figures.

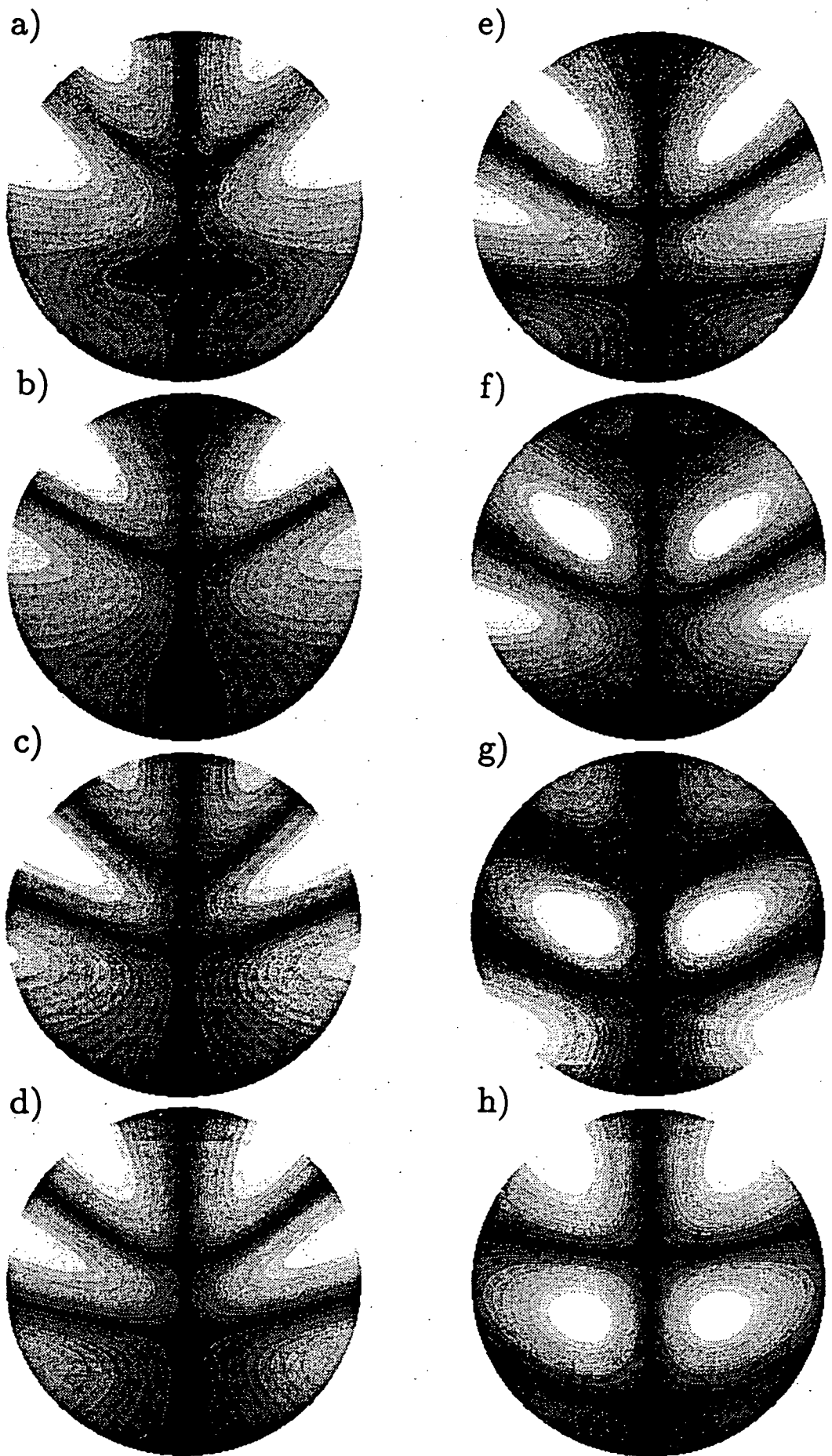


Figure 3.11: Conoscopic figures produced by a LC cell with a) $\theta = 10^\circ$, b) $\theta = 20^\circ$, c) $\theta = 30^\circ$, d) $\theta = 40^\circ$, e) $\theta = 50^\circ$, f) $\theta = 60^\circ$, g) $\theta = 70^\circ$ and h) $\theta = 80^\circ$. As the tilt angle increases the 1λ isochrome and then the optic axis enter the field of view from the top and finally the 2λ isochrome leaves the bottom of the field of view.

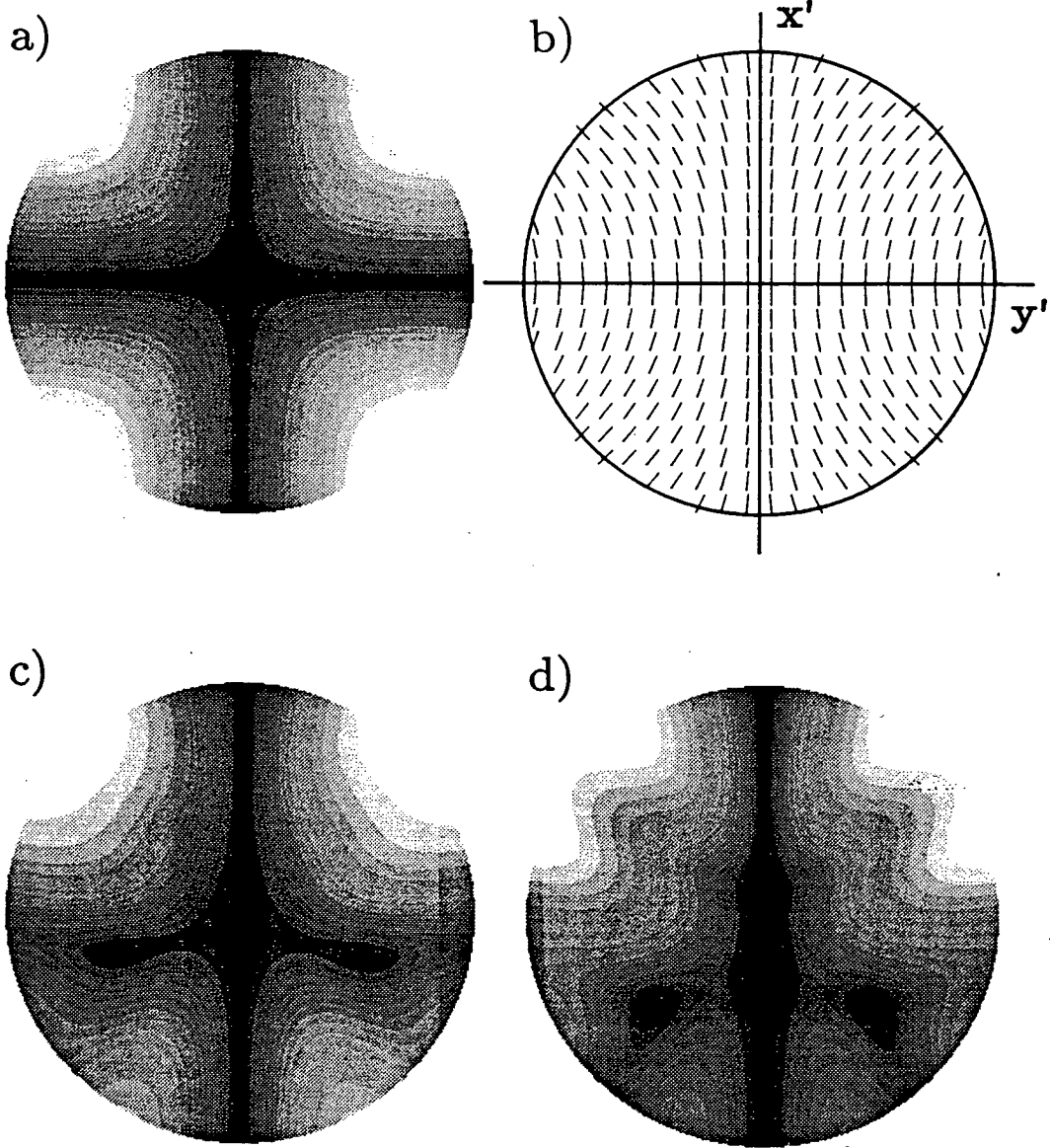


Figure 3.12: a) The isotropic cross produced by a pair of the triplet lenses shown in figure 3.5 when the LC cell is removed. This figure is a result of the lens induced polarisation rotation shown (exaggerated by a factor of four) in b). When the lens induced polarisation is taken into account the conoscopic figures are altered as shown in c) for $\theta = 5^\circ$ (cf figure 3.8a) and d) for $\theta = 10^\circ$ (cf figure 3.11a).

3.5 Conoscopic Measurements

In a SmC* liquid crystal the molecules form a layered structure and tilt away from the layer normal by a constant angle (typically $20 - 25^\circ$) [52]. Within each layer the molecular orientation has a well-defined mean, the director, which at optical frequencies coincides with the uniaxial optic axis [53]. The molecules' transverse dipoles are aligned perpendicular to the director and to the layer normal so that there is a spontaneous polarisation within each layer. As a result of the chirality of the SmC* LC molecules the director and the spontaneous polarisation precess from layer to layer along the layer normal with a helical pitch of order $10\mu\text{m}$ (cf figure 4.1). However when the LC is confined between polymer-coated glass plates with a separation less than the helical pitch the helical structure is unable to form and the LC is optically uniform and ferroelectric. The rôle of the polymer coating is to produce director alignment parallel to the surfaces as in nematic LC devices [41, chapter 3]. Confined in this way the LC director configuration through the cell is uniform to within a couple of degrees (see chapter 4 or reference [52]) and occupies one of two stable states. In one the spontaneous polarisation is pointing partially upwards and in the other partially downwards. Switching between the two states is accomplished by applying a voltage across transparent conducting layers of indium tin oxide (ITO) sandwiched between the polymer and glass layers of the cell. The switching process occurs rapidly ($< 100\mu\text{s}$) because of the strong coupling between the electric field and the spontaneous polarisation.

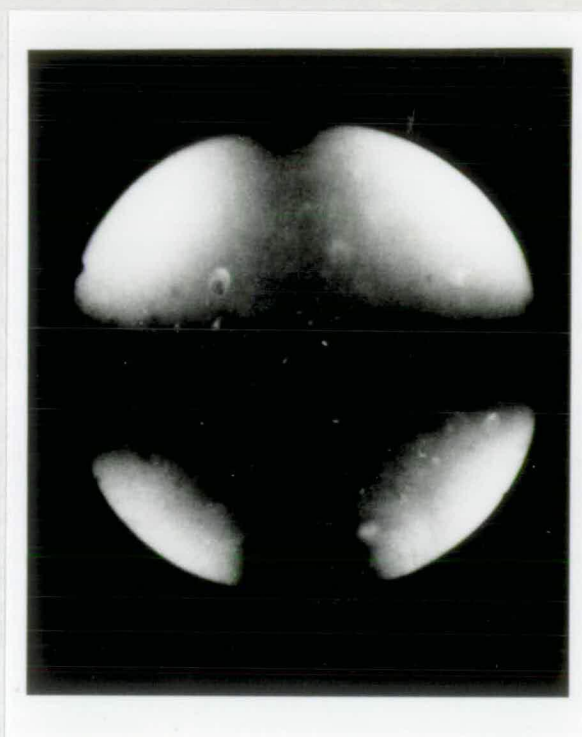
A $7\mu\text{m}$ cell containing the SmC* liquid crystal SCE3 (B.D.H. Limited) was supplied by S.T.C. Technology Limited with nylon alignment layers, a microscope slide as the bottom surface of the cell and a microscope cover-slip as the top surface. This allowed conoscopic examination using microscope objectives with working distances as short as 0.1mm . No ITO coatings were included as only the zero-field conoscopic figures were required. Photographs were taken with

a camera mounted on a Leitz Ortholux 2 Pol.-Ek. polarising microscope fitted with a $50\times$ objective lens of numerical aperture 0.85 (equivalent to a cone angle $\chi = 58.2^\circ$) and a white light source. Figure 3.13a shows the zero-twist ($\phi' = 0$) conoscopic figure produced by the cell described above. In this photograph the isogyre was made more distinct by increasing the contrast during the film development and printing. The figure indicates, by the asymmetry of the cross, that there must be a small director-tilt in the cell. A set of conoscopic figures was calculated, using the data in table 3.1, for tilt angles of 0° to 5° in 1° steps and a cone angle of 58.2° . By comparing these figures with figure 3.13a the director tilt angle was found to be $2^\circ \pm 1^\circ$ in good agreement with calculated director structures [52]. Figure 3.13b and c show the calculated conoscopic figures with (b) and without (c) histogram equalisation for $\theta = 2^\circ$. The theoretical and experimental figures appear rather different because of the different image-processing techniques employed but in both cases the isogyre positions are clearly visible.

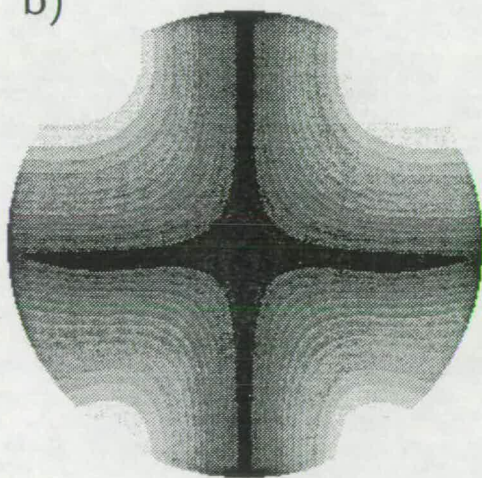
3.6 Conclusions

The model presented in this paper allows rapid and realistic computation of conoscopic figures produced by cells containing homogeneously aligned LC. Image enhancement of the calculated figures shows the location of the isochromes and isogyres precisely although they would normally be indistinct for a sample of the thickness commonly used in LC cells. Comparison of the figures with the intersections of the LC surface and Bertin's surfaces shows the importance of refraction in determining conoscopic figures. Through the introduction of a model of the microscope condenser and objective lens systems the degree of lens-induced polarisation is estimated and this effect is included in the conoscopic calculations. The practical use of the model is demonstrated by its application to a $7\mu\text{m}$ thick cell containing the SmC^* liquid crystal SCE3. The director tilt is determined by comparing the isogyre position in the ex-

a)



b)



c)

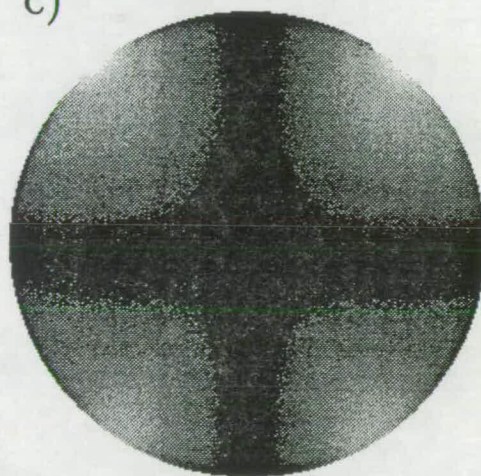


Figure 3.13: a) Conoscopic figure produced by a $7\mu\text{m}$ thick layer of SmC* LC. This figure was compared with calculated conoscopic figures with tilt angles of 0° to 5° in 1° steps. The closest match was with the 2° tilt figure shown in b) image processed and c) as calculated.

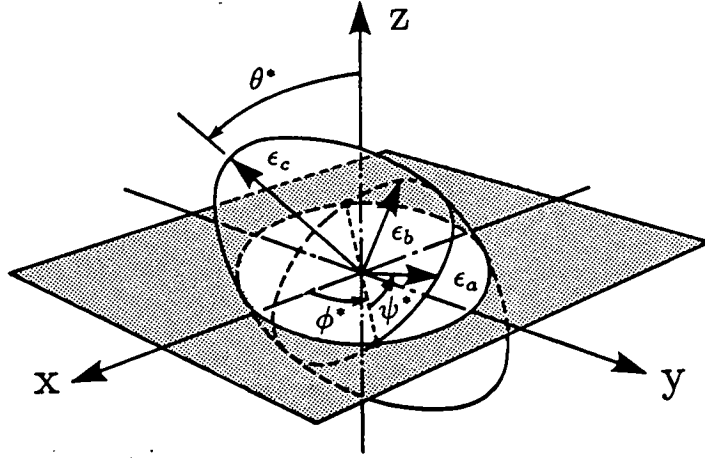


Figure 3.14: The Euler angles (θ^* , ϕ^* and ψ^*) define the orientation of the optical dielectric ellipsoid which has principal semi-axes ϵ_a , ϵ_b and ϵ_c .

perimentally measured conoscopic figure with the positions in the calculated figures. In this way the conoscopic technique may be used quantitatively for any director-orientation. A useful extension of this work would be to calculate the conoscopic figures produced by non-uniform director structures using one of the methods referred to in section 3.2.1. This would provide a useful check on the form of any calculated director structures.

3.7 Appendix A: Derivation of the Wave Vectors

Consider a general anisotropic dielectric medium with principal dielectric tensor components ϵ_a , ϵ_b and ϵ_c subtending Euler angles θ^* , ϕ^* and ψ^* with respect to the xyz coordinate system (see reference [54, chapter 4] and figure 3.14). In a uniaxial medium $\epsilon_a = \epsilon_b$ so the angle ψ^* may be chosen arbitrarily. Let us define $\theta = 90^\circ - \theta^*$ and $\phi = \phi^* - 90^\circ$ as in figure 3.2 and set $\psi^* = 90^\circ$. The rotation

matrix which relates the components of a vector in the dielectric ellipsoid frame to those in the xyz reference frame is then [54, chapter 4]:

$$\mathcal{M} = \begin{pmatrix} -\sin \theta \cos \phi & \sin \phi & \cos \theta \cos \phi \\ -\sin \theta \sin \phi & -\cos \phi & \cos \theta \sin \phi \\ \cos \theta & 0 & \sin \theta \end{pmatrix}. \quad (3.32)$$

This matrix relates two orthogonal coordinate systems, so $\mathcal{M}^{-1} = \mathcal{M}^T$. In the dielectric ellipsoid frame of reference the ordinary and extraordinary wave vectors are

$$(\mathbf{K}_o)_{ell} = \mathcal{M}^T \mathbf{K}_o = (K_{oz} \cos \theta - \beta \sin \theta \sin \phi, -\beta \cos \phi, K_{oz} \sin \theta + \beta \cos \theta \sin \phi)^T, \quad (3.33)$$

$$(\mathbf{K}_e)_{ell} = \mathcal{M}^T \mathbf{K}_e = (K_{ez} \cos \theta - \beta \sin \theta \sin \phi, -\beta \cos \phi, K_{ez} \sin \theta + \beta \cos \theta \sin \phi)^T. \quad (3.34)$$

Maxwell's equations require [44, chapter 9.5] that $(\mathbf{K}_o)_{ell}$ and $(\mathbf{K}_e)_{ell}$ satisfy

$$\frac{K_o^2}{n_o^2} = \frac{\omega^2}{c^2}, \quad (3.35)$$

$$\frac{K_{ea}^2 + K_{eb}^2}{n_e^2} + \frac{K_{ec}^2}{n_o^2} = \frac{\omega^2}{c^2}, \quad (3.36)$$

where $K_o = |(\mathbf{K}_o)_{ell}|$ and K_{ea}, K_{eb} and K_{ec} are the components of $(\mathbf{K}_e)_{ell}$ along the axes of the dielectric ellipsoid. Substituting 3.33 into 3.35 we obtain the two solutions

$$K_{oz} = \pm \sqrt{\left(\frac{n_o \omega}{c}\right)^2 - \beta^2}, \quad (3.37)$$

the positive and negative solutions corresponding to the z -components of the forward and backward propagating ordinary waves, K_{oz} and K'_{oz} , respectively. Substituting 3.34 into 3.36 we obtain, after rearrangement, the two solutions

$$K_{ez} = -\beta \frac{\epsilon_{13}}{\epsilon_{33}} \pm \frac{(\epsilon_{||}\epsilon_{\perp})^{\frac{1}{2}}}{\epsilon_{33}} \sqrt{\epsilon_{33} \left(\frac{\omega}{c}\right)^2 - \beta^2 \left(1 - \frac{\Delta\epsilon}{\epsilon_{||}} \cos^2 \theta \cos^2 \phi\right)} \quad (3.38)$$

where

$$\epsilon_{13} = \Delta\epsilon \sin \theta \cos \theta \sin \phi,$$

$$\begin{aligned}
\epsilon_{33} &= \epsilon_{\perp} + \Delta\epsilon \sin^2 \theta, \\
\Delta\epsilon &= \epsilon_{\parallel} - \epsilon_{\perp}, \\
\epsilon_{\parallel} &= n_e^2, \\
\epsilon_{\perp} &= n_o^2.
\end{aligned}$$

When the positive and negative roots are taken, the solutions correspond to the z -components of the forward and backward propagating extraordinary waves, K_{ez} and K'_{ez} , respectively.

3.8 Appendix B: Derivation of the Electric Vector Directions

Let us define the vectors $\hat{\mathbf{s}}_o$ and $\hat{\mathbf{s}}_e$ as follows:

$$\hat{\mathbf{s}}_o = (\mathbf{K}_o)_{ell} / |\mathbf{K}_o| = (s_{oa}, s_{ob}, s_{oc})^T, \quad (3.39)$$

$$\hat{\mathbf{s}}_e = (\mathbf{K}_e)_{ell} / |\mathbf{K}_e| = (s_{ea}, s_{eb}, s_{ec})^T. \quad (3.40)$$

Yeh [44, chapter 9.2] has shown that the electric-field-vector directions are given by

$$(\hat{\mathbf{o}})_{ell} = (s_{ob}, -s_{oa}, 0)^T, \quad (3.41)$$

$$(\hat{\mathbf{e}})_{ell} = \left(\frac{s_{ea}}{n_e^2(\chi_e) - n_o^2}, \frac{s_{eb}}{n_e^2(\chi_e) - n_o^2}, \frac{s_{ec}}{n_e^2(\chi_e) - n_e^2} \right)^T, \quad (3.42)$$

$$(3.43)$$

where the refraction angle χ_e is given by equation 3.14 and $n_e(\chi_e)$ by equation 3.15. Substituting equations 3.39 and 3.40 into equations 3.41 and 3.42 we find

$$(\hat{\mathbf{o}})_{ell} = N_o(-\beta \cos \phi, \beta \sin \theta \sin \phi - K_{oz} \cos \theta, 0)^T, \quad (3.44)$$

$$(\hat{\mathbf{e}})_{ell} = N_e \left(\frac{K_{ex} \cos \theta - \beta \sin \theta \sin \phi}{n_e^2(\chi_e) - n_o^2}, \frac{-\beta \cos \phi}{n_e^2(\chi_e) - n_o^2}, \frac{K_{ex} \sin \theta + \beta \cos \theta \sin \phi}{n_e^2(\chi_e) - n_e^2} \right)^T, \quad (3.45)$$

where N_o and N_e are normalising constants. In the xyz frame of reference the vectors $\hat{\mathbf{o}}$ and $\hat{\mathbf{e}}$ are therefore given by

$$\hat{\mathbf{o}} = \mathcal{M}(\hat{\mathbf{o}})_{ell}, \quad (3.46)$$

$$\hat{\mathbf{e}} = \mathcal{M}(\hat{\mathbf{e}})_{ell}. \quad (3.47)$$

Chapter 4

A Method for Computing the Optical Properties of a Smectic C* Liquid Crystal Cell

4.1 Introduction to SmC* LCs

Ferroelectricity in LCs was first observed and explained by Meyer *et al.* [55] in the SmC* and SmH phases (see chapter 1 for details of the various smectic phases). Recently interest has focussed on the SmC* phase and a wide range of electro-optic light modulators including high resolution flat panel displays[56] and spatial light modulators[57] has been built. These devices, unlike those containing nematic LC, do not require an active matrix[58] (where each pixel has its own curcuitry) because of the bistability of the eletro-optic effect used in them. A large proportion of previous work on ferroelectric LCs, both theoretical and experimental, has been with LC cells of thickness $2\mu m$ or less. There have been two reasons for using such thin cells: first that the surface interactions, which make the device optically uniform, are most effective in thin cells and second that LC layers of this thickness approximately satisfy the condition for maximum contrast between the two stable states of the LC (see section 4.6). However it is much easier to build thicker cells reliably and it might be possible to use the same production lines as for nematic LC displays. In this chapter a

formalism is developed to describe thicker ($7\mu m$) cells and the formalism is used to examine some of their advantages and disadvantages relative to thin cells. This formalism takes into account interactions within and between the smectic layers which have not been considered in previous work.

Smectic LCs are characterised by orientational order and varying degrees of positional order of their molecules. In a chiral smectic C (SmC^*) LC the molecules form a layered structure and tilt away from the layer normal by an angle θ (cf figure 4.1). The director, a unit vector $\mathbf{n}$, is defined as being the local mean molecular orientation and the projection of this director onto the layer plane defines the orientation of the unit length $\mathbf{c}$ -director. In order to maintain the minimum-energy configuration, in which the smectic layers have constant spacing, the $\mathbf{n}$ -director may only move on the surface of a cone. As a result of the chirality of the SmC^* molecules the $\mathbf{n}$ -director precesses about the cone from layer to layer. In addition the chirality reduces molecular symmetry within each layer in such a way as to align the molecules' transverse dipoles[59, chapter 7]. The resultant spontaneous polarisation $\mathbf{P}_s$ lies perpendicular to the $\mathbf{c}$ -director and in the layer plane as shown in figure 4.1. Thus, within each layer, SmC^* LCs are ferroelectric though the orientation of $\mathbf{P}_s$ precesses from layer to layer.

SmC^* liquid crystals, though biaxial, are to a good approximation[60] uniaxial at optical frequencies. The $\mathbf{n}$ -director is parallel to the local optic axis of the medium. In order to produce a uniform electro-optic effect the helical structure must first be unwound. Clark and Lagerwall[61] first did this using the so-called surface stabilised ferroelectric LC (SSFLC) geometry in which the LC is sandwiched between two glass plates spaced approximately $1\mu m$ apart as shown in figure 4.2. In this geometry the LC has two stable director configurations one with $\mathbf{P}_s$ pointing up and the other with $\mathbf{P}_s$ pointing down. Bistable switching from one to the other is achieved by applying a d.c. voltage pulse across the indium tin oxide (ITO) electrodes. Optical contrast is produced by placing the LC cell between crossed polaroids and aligning the $\mathbf{n}$ -director of one state with

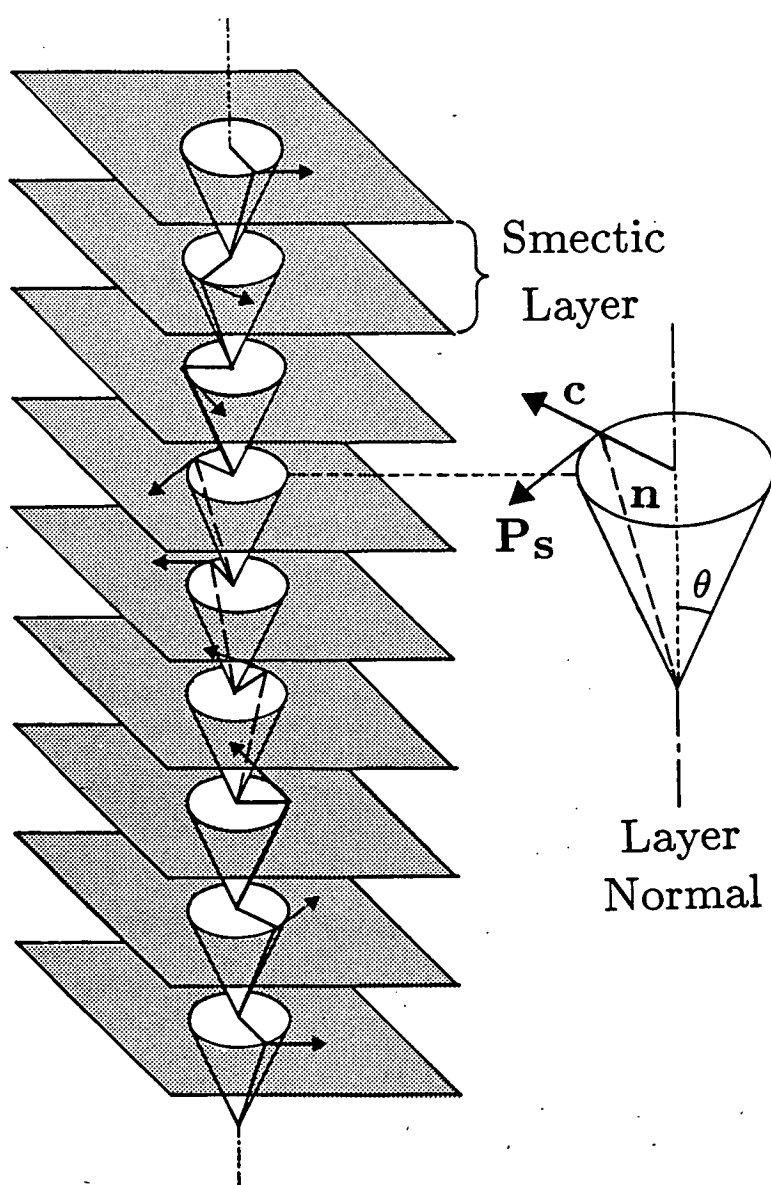


Figure 4.1: Director configuration in a bulk sample of SmC* LC. Within each smectic layer the $\mathbf{n}$ -director makes a constant angle θ with the layer normal and precesses about the layer normal from layer to layer. The spontaneous polarisation $\mathbf{P}_s$ lies in the smectic layer plane and perpendicular to the projection of the $\mathbf{n}$ -director onto the plane. This projected direction also defines the $\mathbf{c}$ -director orientation.

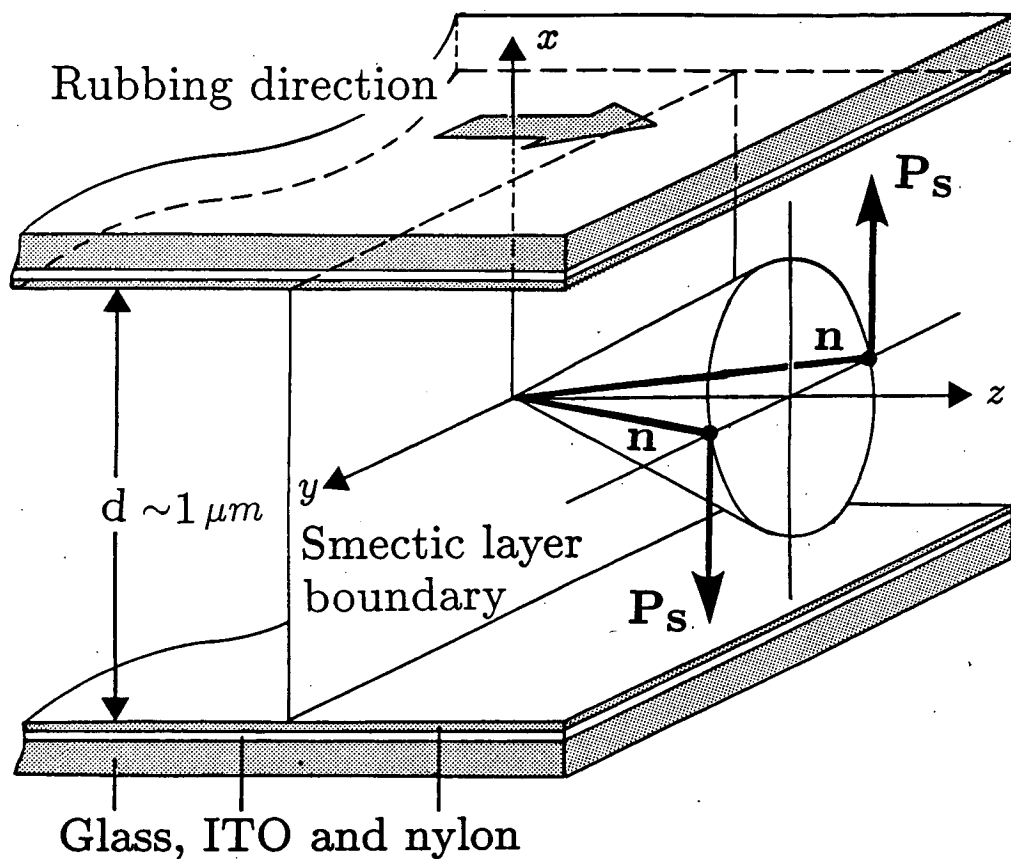


Figure 4.2: Ideal SSFLC cell. Provided that the cell thickness is small compared with the pitch length of the helix shown in figure 4.1 the helix is prevented from forming by surface forces. The n -director takes up one of the two stable orientations shown, symmetrically positioned on either side of the rubbing direction. If a d.c. voltage is applied across the cell the n -director can be switched from one orientation to the other.

the axis of the front polariser.

SSFLC devices have switching times several orders of magnitude faster than the best nematic LC devices; this is because in the ferroelectric devices the electric field couples directly to the spontaneous polarisation whereas in the nematic devices the field interacts with the dielectric anisotropy of the medium. SmC* LCs do have a dielectric anisotropy but the interaction of the electric field with the spontaneous polarisation is much stronger for typical device voltages ($< 20V$) than the interaction with the dielectric anisotropy. There are however two major problems with these SmC* devices. First it is difficult to avoid large relative thickness variations of the LC layer when it is so thin and second the LC must have a large birefringence if it is to act as a half-wave plate and so satisfy the condition for optimum contrast (see section 4.6 and [62, chapter 14.4]). If thicker cells are used then both of these restrictions may be relaxed, although thicker cells suffer from less effective surface stabilisation. In this chapter the director configurations which occur in thicker cells are calculated and used to investigate how the behaviour of a thick cell differs from that described above.

Elastic continuum theories have been used widely in the study of both nematic and smectic liquid crystals. Minimisation of the free energy functions generated by these theories makes it possible to calculate the director configurations. A survey of the functions which have been used to describe SmC* LCs was provided by Akahane and Nakagawa[63]. In all of the expressions given however the smectic layers were assumed to be planar, either perpendicular to the glass surfaces or tilted at a constant angle to them. *A priori* there is no reason why these layers should have a fixed orientation or indeed be planar at all. de Gennes[59, chapter 7] has derived a general expression for the free energy density of SmC* LCs which takes account of layer distortions as well as director distortions within layers. In this chapter we compute the director configuration in a $7\mu m$ thick cell, using de Gennes' expression, as reformulated by Dahl and Lagerwall[64, equations 7 – 11], along with an improved form of surface interac-

tion energy function. As far as the author knows this is the first time that Dahl and Lagerwall's energy expression has been investigated in its full form. The method we used to find the minimum-energy configuration takes into account the contribution of the polarisation field to the local electric field and the way in which this local field interacts with both the spontaneous and the induced polarisations of the molecules. The transmittance of a $7\text{ }\mu\text{m}$ thick cell for different azimuthal orientations of the cell between crossed polarisers is then computed by using the 4×4 matrix method of Berreman (see section 2.9 and reference [65]). The theoretical and measured azimuthal orientations which give minimum transmittance are shown to be in good agreement. Finally it is shown that the computed-average-tilt angle is consistent with conoscopic measurements performed with a polarising microscope.

4.2 A General Theory of SmC* LCs

In this section the equations used to describe the free energy of bulk LC distortions, surface interactions and field interactions are presented. First, the coordinate system used in the theoretical formulation is shown in figure 4.3. In the xyz coordinate system (figure 4.3a; cf figure 4.2) the x -axis is normal to the bounding plates and the z -axis corresponds to the rubbing direction of the nylon surface treatment (see section 4.5.1 below for details). It is observed experimentally that the two stable states of the LC are symmetrically positioned about the xz -plane. Therefore it is assumed that the unit vector $\hat{\mathbf{k}}$, describing the layer normal at any point, can be uniquely described by the angle ψ (figure 4.3b). This angle relates the xyz coordinate system to the $x'yz'$ system in which the c -director orientation is specified by the angle ϕ (figure 4.3c). It is also assumed that, since the LC cell described in section 4.5.1 appeared uniform in optical texture, c and $\mathbf{k}$ varied only in the x -direction. In the xyz coordinate system

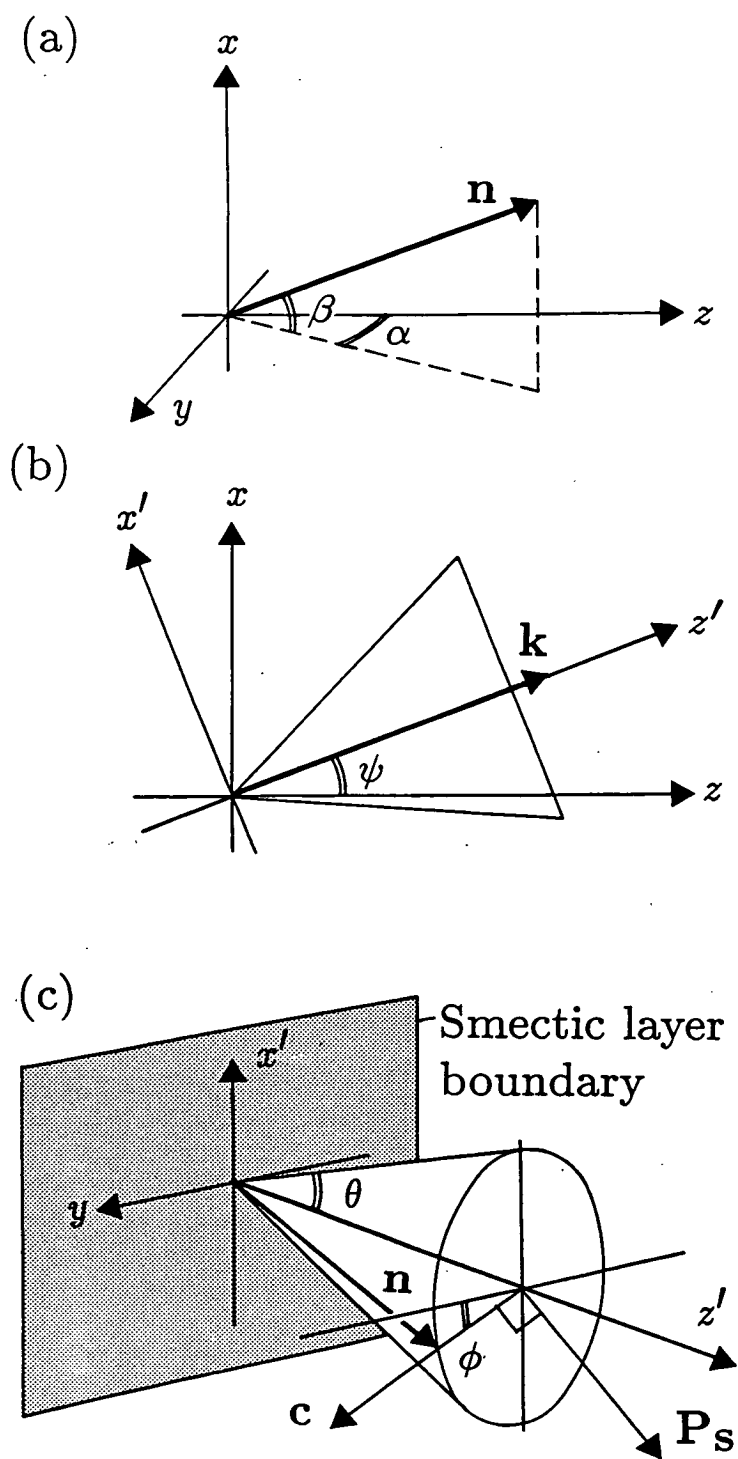


Figure 4.3: Coordinate system used in the theoretical formulation to describe the director orientation.

the $\mathbf{c}$ and $\mathbf{k}$ vectors are given by

$$\mathbf{c} = (-\cos \psi \sin \phi, \cos \phi, \sin \psi \sin \phi), \quad (4.1)$$

$$\mathbf{k} = (\sin \psi, 0, \cos \psi). \quad (4.2)$$

These vectors are orthonormal and together describe all possible director orientations. The two angles ϕ and ψ also uniquely define the director orientations. Within this coordinate system the unit vector $\mathbf{p}$ defining the direction of the spontaneous polarisation $\mathbf{P}_s$ is given by

$$\mathbf{p} = \mathbf{k} \times \mathbf{c}. \quad (4.3)$$

Using the definitions 4.1 and 4.2 allows us to compute $\mathbf{n}$ with the following expression

$$\mathbf{n} = \mathbf{k} \cos \theta + \mathbf{c} \sin \theta. \quad (4.4)$$

Equation 4.4 then allows us to compute the tilt angle β and the azimuthal angle α thus:

$$\sin \beta = n_x = \sin \psi \cos \theta - \cos \psi \sin \phi \sin \theta, \quad (4.5)$$

$$\sin \alpha = \frac{n_y}{\cos \beta} = \frac{\cos \phi \sin \theta}{\cos \beta}. \quad (4.6)$$

These coordinate systems enable us to derive the appropriate form for the free energy density. de Gennes[59, chapter 7] has derived a general expression for the elastic free energy density, f_{elas} , of a SmC* LC. This expression was reformulated by Dahl and Lagerwall[64] in terms of the vectors $\mathbf{c}$ and $\mathbf{k}$ thus:

$$f_{elas} = f_c + f_s + f_{cs} + f_*. \quad (4.7)$$

where f_c is the contribution from $\mathbf{c}$ -director distortions, f_s is from the layer distortions, f_{cs} is from the coupling between $\mathbf{c}$ -director and layer distortions and f_* is the chiral elastic contribution. In the above expression

$$f_c = \frac{1}{2}B_1[\mathbf{k} \cdot (\nabla \times \mathbf{c})]^2 + \frac{1}{2}B_2(\nabla \cdot \mathbf{c})^2 + \frac{1}{2}B_3\{\mathbf{c} \cdot [\nabla \times \mathbf{c} + (\nabla \cdot \mathbf{k})(\mathbf{k} \times \mathbf{c})]\}^2 - B_{13}[\mathbf{k} \cdot (\nabla \times \mathbf{c})]\{\mathbf{c} \cdot [\nabla \times \mathbf{c} + (\nabla \cdot \mathbf{k})(\mathbf{k} \times \mathbf{c})]\}, \quad (4.8)$$

$$f_s = \frac{1}{2}A_{11}[\mathbf{c} \cdot (\nabla_s \mathbf{k}) \cdot (\mathbf{k} \times \mathbf{c})]^2 + \frac{1}{2}A_{12}[\mathbf{c} \cdot (\nabla_s \mathbf{k}) \cdot \mathbf{c}]^2 + \frac{1}{2}A_{21}[(\mathbf{k} \times \mathbf{c}) \cdot (\nabla_s \mathbf{k}) \cdot (\mathbf{k} \times \mathbf{c})]^2, \quad (4.9)$$

$$f_{cs} = -C_1[\mathbf{c} \cdot (\nabla_s \mathbf{k}) \cdot (\mathbf{k} \times \mathbf{c})][\mathbf{k} \cdot (\nabla \times \mathbf{c})] - C_2[(\mathbf{k} \times \mathbf{c}) \cdot (\nabla_s \mathbf{k}) \cdot (\mathbf{k} \times \mathbf{c})](\nabla \cdot \mathbf{c}), \quad (4.10)$$

$$f_* = D_1 \mathbf{k} \cdot (\nabla \times \mathbf{c}) - D_2 \mathbf{c} \cdot (\nabla_s \mathbf{k}) \cdot (\mathbf{k} \times \mathbf{c}) - D \mathbf{c} \cdot [\nabla \times \mathbf{c} + (\nabla_s \mathbf{k}) \cdot (\mathbf{k} \times \mathbf{c})] \quad (4.11)$$

and $\nabla_s \mathbf{k}$ is the symmetric part of the tensor $\nabla \mathbf{k}$. In equation 4.8 the B_1, B_2 and B_3 terms correspond to bend, splay and twist distortions (see section 2.2) of the $\mathbf{c}$ -director while the B_{13} term corresponds to the coupling between bend and twist distortions of the $\mathbf{c}$ -director. The A and C constants in equations 4.9 and 4.10 correspond to layer distortions and coupling between $\mathbf{c}$ -director distortions and layer distortions respectively. In equation 4.11 the D term is associated with the $\mathbf{c}$ -director twist shown in figure 4.1, the D_1 term represents a tendency to produce a constant bend of the $\mathbf{c}$ -director and the D_2 term couples $\mathbf{c}$ -director twist to layer bending. Values of these elastic constants can be estimated in terms of the Frank elastic constants of nematic theory and the helical pitch of the $\mathbf{c}$ -director in a bulk LC sample as shown in section 4.3.2.

Substituting equations 4.1 and 4.2 into equations 4.8 to 4.11 we have obtained the following expressions for the case in which ϕ and ψ are functions of x only:

$$f_c = \frac{1}{2}B_1(\phi_x \cos \psi \sin \phi)^2 + \frac{1}{2}B_2(\psi_x \sin \psi \sin \phi - \phi_x \cos \psi \cos \phi)^2 + \frac{1}{2}B_3(\phi_x \sin \psi)^2 - B_{13}\phi_x^2 \cos \psi \sin \psi \sin \phi, \quad (4.12)$$

$$f_s = \frac{1}{2}A_{11}(\psi_x \cos \psi \cos \phi \sin \phi)^2 + \frac{1}{2}A_{12}(\psi_x \cos \psi \sin^2 \phi)^2 + \frac{1}{2}A_{21}(\psi_x \cos \psi \cos^2 \phi)^2, \quad (4.13)$$

$$f_{cs} = C_1 \psi_x \phi_x \cos^2 \psi \cos \phi \sin^2 \phi - C_2 \psi_x \cos \psi \cos^2 \phi (\psi_x \sin \psi \sin \phi - \phi_x \cos \psi \cos \phi), \quad (4.14)$$

$$f_* = D \phi_x \sin \psi - D_1 \phi_x \cos \psi \sin \phi - D_2 \psi_x \cos \psi \cos \phi \sin \phi, \quad (4.15)$$

where each subscript x denotes the operation $\partial/\partial x$.

Next we consider the contribution to the free energy density arising from the interaction of the LC with a static electric field. The contribution associated with the induced dipoles, the dielectric free energy density, is given by

$$f_d = -\frac{1}{2}\epsilon_{xx} \left(\frac{\partial \Phi}{\partial x} \right)^2 \quad (4.16)$$

where Φ is the electric scalar potential which is related to the x -component of the electric field by $E_x = -\partial \Phi / \partial x$. ϵ_{xx} is the component of the dielectric ellipsoid parallel to the x -axis which is given[66] by

$$\epsilon_{xx} = \epsilon_o \epsilon_{\perp} (1 + e \sin^2 \beta) \quad (4.17)$$

where $e = (\epsilon_{\parallel} - \epsilon_{\perp}) / \epsilon_{\perp}$ and $\epsilon_{\parallel}$ and $\epsilon_{\perp}$ are the principal dielectric constants along the $\mathbf{n}$ -director and perpendicular to it. The contribution to the free energy density associated with the interaction of the electric field $\mathbf{E}$ with the spontaneous polarisation $\mathbf{P}_s$ is given by

$$f_p = -P_s \cos \psi \cos \phi \left(\frac{\partial \Phi}{\partial x} \right). \quad (4.18)$$

Finally we consider the contribution to the total free energy arising from the interaction of the LC with its bounding surfaces. Two terms are considered: the first is of the general type used by Nakagawa *et al.* [66] which has two energy minima for ϕ , one on either side of $\phi = \pi/2$, and the second is a nematic type of surface interaction which has energy minima for $\beta = 0$ and $\beta = \pi$. Together they encourage a uniform layer tilt across the cell with the surface $\mathbf{n}$ -director parallel to the surface in one of two positions symmetrically positioned either side of the rubbing direction. A tilted layer formation is thought to be produced by the layer shrinkage which occurs as the LC cools from the smectic A phase to the SmC* phase [67].

We shall assume that the surface free energy per unit area is

$$f_{sur} = -\sigma_1 f_1(\phi) - \sigma_2 f_2(\beta) \quad (4.19)$$

where

$$f_1(\phi) = \begin{cases} \exp \left[-\gamma \sin^2 \left(\frac{\phi_1}{2} \right) \right] & \text{if } \phi \notin [2m\pi + \phi_o, (2m+1)\pi - \phi_o] \\ \left(\frac{\pi - 2\phi_o}{\pi + 2\phi_o} \right) \sin^2 \phi_2 & \text{otherwise,} \end{cases}$$

where

$$\begin{aligned} \phi_1 &= \left(\frac{2\pi}{\pi + 2\phi_o} \right) [\phi - ((2m+1)\pi - \phi_o)], \\ \phi_2 &= \left(\frac{\pi}{\pi - 2\phi_o} \right) [\phi - (2m\pi + \phi_o)] \end{aligned}$$

and

$$f_2(\beta) = \exp(-\gamma \sin^2 \beta). \quad (4.20)$$

In the above equations m is any integer, γ is a constant which controls the steepness of the potential wells in the surface-potential functions and ϕ_o defines the positions of the minima in $f_1(\phi)$. Figure 4.4 shows the form these functions take for some typical values of γ and ϕ_o . The value of ϕ_o was determined approximately from experimental measurements (cf section 4.5.1) of the zero-field apparent azimuthal angle using equation 4.6 and assuming no surface pretilt i.e. $\beta = 0$. Although the mathematical form of f_{sur} is not derived physically it does reproduce the tilted layer formation which is thought to occur [67] and is therefore used as a first approximation. The total free energy is thus given by

$$\begin{aligned} F(\phi, \psi; \Phi) &= \int_v f_{vol} dv + \int_s f_{sur} ds \\ &= \int_v (f_{elas} + f_d + f_p) dv + \int_s f_{sur} ds. \end{aligned} \quad (4.21)$$

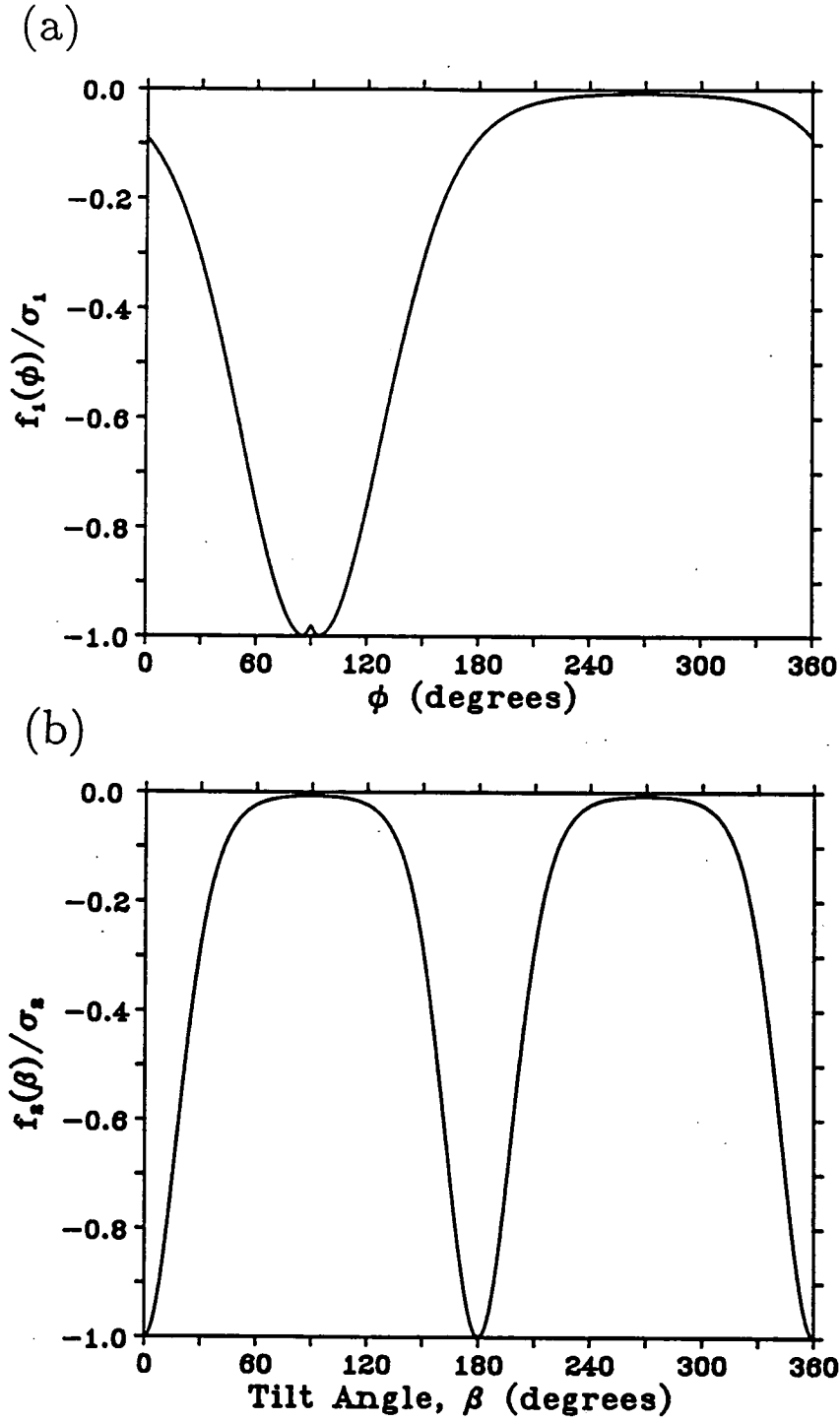


Figure 4.4: Form of the surface-interaction potentials a) $f_1(\phi)/\sigma_1$, and b) $f_2(\beta)/\sigma_2$, with $\gamma = 5$ and $\phi_o = 86.5^\circ$. γ controls the steepness of the potential wells and ϕ_o controls the positions of the minima in $f_1(\phi)$. The combined effect of the potentials is to produce uniformly tilted layers when no voltage is applied.

4.3 Calculating the Minimum-Energy Director Configuration

4.3.1 Minimising the Free Energy Function

In this section we solve the free energy equation 4.21 to find the minimum energy director configuration. Although we are concerned only with static director configurations it is convenient to introduce pseudo viscosities for the rotations of $\mathbf{c}$ and $\mathbf{k}$. A time-dependent formulation of the solution was chosen because the associated iteration method is stable for any combination of elastic constants. However it may be possible to interpret the pseudo viscosities as real viscosities and calculate dynamic director configurations [66]. The bulk torque balance equations can then be written as

$$\eta_v \frac{\partial \phi}{\partial t} = - \left[\frac{\partial f_{\text{vol}}}{\partial \phi} - \frac{\partial}{\partial x} \left(\frac{\partial f_{\text{vol}}}{\partial \phi_x} \right) \right], \quad (0 < x < d), \quad (4.22)$$

$$\eta_v \frac{\partial \psi}{\partial t} = - \left[\frac{\partial f_{\text{vol}}}{\partial \psi} - \frac{\partial}{\partial x} \left(\frac{\partial f_{\text{vol}}}{\partial \psi_x} \right) \right], \quad (0 < x < d). \quad (4.23)$$

The surface torque balance equations are

$$\eta_s \frac{\partial \phi}{\partial t} = - \left[\frac{\partial f_{\text{surf}}}{\partial \phi} - (\mathbf{x} \cdot \mathbf{s}) \frac{\partial f_{\text{surf}}}{\partial \phi_s} \right], \quad (x = 0, d), \quad (4.24)$$

$$\eta_s \frac{\partial \psi}{\partial t} = - \left[\frac{\partial f_{\text{surf}}}{\partial \psi} - (\mathbf{x} \cdot \mathbf{s}) \frac{\partial f_{\text{surf}}}{\partial \psi_s} \right], \quad (x = 0, d). \quad (4.25)$$

Equations 4.22 to 4.25 are in the form of multi-variable TDGL (time dependent Ginzberg-Landau) equations [68]. In the equations η_v is the bulk rotational viscosity of both $\mathbf{c}$ and $\mathbf{k}$ and η_s is the surface rotational viscosity. The $\mathbf{c}$ and $\mathbf{k}$ viscosities are assumed to be equal for convenience but in general would be different. In equations 4.24 and 4.25 $\mathbf{s}$ is the unit surface normal pointing into the LC at each surface and $\mathbf{x}$ is the unit vector in the x -direction. In the torque-balance equations the terms involving the viscosities vanish for the steady-state solutions and the values of the viscosities simply control the rate of convergence to that solution. Substituting equation 4.21 into equations 4.22 to 4.25 we have

obtained the following simultaneous coupled partial differential equations:

$$\eta_v \frac{\partial \phi}{\partial t} = -(\Gamma_1 \phi_{xx} + \Gamma_2 \psi_{xx} + \Gamma_3 \phi_x^2 + \Gamma_4 \psi_x^2 + \Gamma_5 \psi_x \phi_x + \Gamma_6 \psi_x + \Gamma_7), \quad (4.26)$$

$$\eta_v \frac{\partial \psi}{\partial t} = -(\Lambda_1 \psi_{xx} + \Lambda_2 \phi_{xx} + \Lambda_3 \phi_x^2 + \Lambda_4 \psi_x^2 + \Lambda_5 \psi_x \phi_x + \Lambda_6 \phi_x + \Lambda_7), \quad (4.27)$$

$$\eta_s \frac{\partial \phi}{\partial t} = (\mathbf{x.s})(\Gamma_8 \phi_x + \Gamma_9 \psi_x + \Gamma_{10}) - \Gamma_{11}, \quad (4.28)$$

$$\eta_s \frac{\partial \psi}{\partial t} = (\mathbf{x.s})(\Lambda_8 \psi_x + \Lambda_9 \phi_x + \Lambda_{10}) - \Lambda_{11}. \quad (4.29)$$

The forms of the Γ_i and Λ_i are given in appendix A.

To solve these equations we must know the local electric field strength within the LC, taking into account the polarisation field produced by the spontaneous polarisation $\mathbf{P}_s$. The polarisation field is particularly important when small external fields are applied, as was shown by Nakagawa *et al.*[69], because it has the effect of reducing the local electric field strength in regions where there is a large rate of change of the orientation of $\mathbf{P}_s$. Introducing a pseudo viscosity η_Φ we can minimise the volume free energy with respect to Φ as for ϕ and ψ . For a particular director configuration, Φ is obtained by finding the steady-state solution of

$$\eta_\Phi \frac{\partial \Phi}{\partial t} = - \left[\frac{\partial f_{\text{vol}}}{\partial \Phi} - \frac{\partial}{\partial x} \left(\frac{\partial f_{\text{vol}}}{\partial \Phi_x} \right) \right], \quad (0 < x < d), \quad (4.30)$$

subject to the boundary conditions that $\Phi(0) = 0$ and $\Phi(d) = V$ (where V is the voltage applied across the cell). Substituting equation 4.21 into equation 4.30 we obtain

$$\eta_\Phi \frac{\partial \Phi}{\partial t} = - \left\{ \frac{\partial}{\partial x} \left[\epsilon_o \epsilon_\perp (1 + e \sin^2 \beta) \frac{\partial \Phi}{\partial x} \right] - P_s (\psi_x \sin \psi \cos \phi + \phi_x \cos \psi \sin \phi) \right\}. \quad (4.31)$$

The solution to this equation shows how the scalar potential varies as a function of x .

In order to calculate the director configuration across the cell we first replace all the derivatives in equations 4.26 to 4.29 and 4.31 by finite differences (see appendix B). To do this we divide the x -axis between $x = 0$ and $x = d$ into N divisions of length $\Delta x = d/N$ and divide time into steps of duration Δt . For a

cell of thickness $7\mu m$, N is set to 72. If we denote a division of the x -axis by Δx then the time division Δt must satisfy certain conditions to ensure convergence of the iterative method[70, chapter 10.2]. Equations 4.26 to 4.29 will converge provided that:

$$\left[\frac{\Delta t}{\eta_v(\Delta x)^2} \right] \max(A_{11}, A_{12}, A_{21}, B_1, B_2, B_3, B_{13}, C_1, C_2) < 0.5 \quad (4.32)$$

where the function $\max$ selects the largest one of its arguments. The bulk rotational viscosity is taken (arbitrarily) to be $10^{-2} Pa.s$ and the time step Δt chosen to make the left-hand-side of equation 4.32 equal to 0.1. η_s , the surface rotational viscosity is taken to be $\eta_v \Delta x$. A necessary condition for the convergence of equation 4.31 is that

$$\frac{\Delta t \epsilon_o \epsilon_{\perp} e}{\eta_{\Phi}(\Delta x)^2} < 0.5 \quad (4.33)$$

so η_{Φ} is chosen to make the left hand side of inequality 4.33 equal to 0.1. Once $\Delta x, \Delta t$ and the viscosities have been selected the starting configuration is chosen to be $\phi(x) = \psi(x) = 0$ for which $\Phi(x) = xV/d$. The fourth order Runge-Kutta method (see appendix B and [70, chapter 9]) is then used to solve equations 4.26 to 4.29. After each time step the scalar potential is evaluated by solving equation 4.31, also using the fourth order Runge-Kutta method.

4.3.2 Estimating Values for the Elastic Constants

In this subsection the method of estimating values for the elastic constants in the free energy equation is explained. A comparison is made between the form of the elastic free energy density used here and an expression resembling a nematic elastic free energy density. The values of the smectic elastic constants are then estimated from typical values of the nematic elastic constants. This comparison requires that the layer normal be constant. It is assumed to be so here for the estimation of the values of the elastic constants but it is allowed to vary subsequently. Handschy *et al.*[71] proposed a simple extension of the nematic

elastic free energy density (see section 2.2) to describe SmC* LCs:

$$f = \frac{1}{2}k_{11}(\nabla \cdot \mathbf{n})^2 + \frac{1}{2}k_{22}(\mathbf{n} \cdot \nabla \times \mathbf{n} + q_{||})^2 + \frac{1}{2}k_{33}(\mathbf{n} \times \nabla \times \mathbf{n} + \mathbf{q}_{\perp})^2, \quad (4.34)$$

where $q_{||}$ denotes the spontaneous twist and the vector $\mathbf{q}_{\perp}$ denotes the spontaneous bend of the $\mathbf{n}$ -director. In this expression k_{11} , k_{22} and k_{33} are the elastic constants associated with splay, twist and bend distortions of the $\mathbf{n}$ -director (see section 2.2). If we assume that k is constant throughout the LC in equation 4.7 and we set $k_{11} = k_{22} = k_{33} = k$ then it can be shown [63] that $B_1 = B_2 = B_3 = k \sin^2 \theta = B$ and $B_{13} = 0$. In a typical nematic LC k is of the order of 10^{-11} N so we expect B to be somewhat greater than 10^{-12} N . It is important to realise that the comparison between nematic and SmC* LCs is only made to obtain an estimate of the order of magnitude of the SmC* elastic constants. When all the k_{ii} constants are set equal, equation 4.34 is minimised for $\phi = q_o z$ where q_o is given [63] by

$$q_o = \frac{-D}{k \sin^2 \theta}. \quad (4.35)$$

In this equation $q_o = 2\pi/p_o$ and p_o is the pitch of the helix shown in figure 4.1. The pitch of the helix can be measured directly (see section 4.5.3) and has a value of $5.8 \mu\text{m}$ for the LC SCE3 at 15°C . Therefore we can estimate the value of D from equation 4.35. The significance of the sign is that it determines the sense in which the helix is wound.

In the following analysis it is assumed that the layer bend elastic constants are all equal and have the same value as the B elastic constants i.e. $A_{11} = A_{12} = A_{21} = B$ and that as a first approximation the C elastic constants can be set to zero. That is to say, equal weight is given to each of the different layer bend and $\mathbf{c}$ -director distortion elastic constants and that all coupling between distortions is ignored. The chiral elastic constants D_1 and D_2 are set equal to the modulus of the value of D computed using equation 4.35. It is also assumed that the surface elastic constants are equal i.e. $\sigma_1 = \sigma_2 = \sigma$. Therefore the entire set of elastic constants can be specified by choosing values of B , σ and γ . For these values

the director configuration is calculated, and from this certain optical properties of the LC cell are obtained as described in the next section. A parameter survey is then performed to find the best fit to the experimentally measured optical properties.

4.4 Calculating LC Cell Optical Properties

This section describes the way in which the theory developed in sections 4.2 and 4.3 is used to simulate some of the optical properties of a SmC* LC cell. The first simulation is trivially performed once the director configuration has been calculated. This simulation consists of calculating the average tilt angle $\bar{\beta}$ and comparing it with the value of $\bar{\beta}$ measured from the conoscopic figure of the cell as described in section 4.5.2. The second simulation permits comparison of the predicted values of the azimuthal angle α with those observed experimentally. In particular a simulation is performed in which the cell is positioned between crossed polaroids and rotated about the x -axis until the minimum-transmission orientation is found. This orientation defines the apparent azimuthal angle α_{app} for the whole cell. The computed variation of α_{app} with voltage is compared with experimentally measured values in order to test the theory further.

The conoscopic image (section 4.5.2) is determined by the effective birefringence of the LC layer and its azimuthal orientation relative to the polariser axis. In a non-uniform sample the conoscopic figure will depend on the birefringence at every point through the sample. The total phase difference introduced along a particular path will be the integral of the phase differences along that path. When no voltage is applied to the LC cell waveguiding (see section 2.1) occurs so that, to a first approximation, there is no mixing of the ordinary and extraordinary waves. Therefore the total phase difference for a particular angle of incidence may be calculated by integrating along the ordinary and extraordi-

nary wave-paths separately and taking the difference of the integrated values. For normally incident light the effective ordinary and extraordinary refractive indices are n_o and [72, chapter 6]

$$n_{eff} = \frac{n_e n_o}{\sqrt{n_e^2 \sin^2 \beta + n_o^2 \cos^2 \beta}} \quad (4.36)$$

where β is the tilt angle and n_e and n_o are the extraordinary and ordinary refractive indices of the medium. A numerical integration is then performed, using the computed values of β , to calculate the total phase difference Δ across the cell. It is assumed that the conoscopic figure which would be produced by the computed director structure would be the same as that produced by a uniform LC layer whose tilt angle $\bar{\beta}$ is chosen to give the same value of Δ for normally incident light. This assumption is reasonable provided that the director distortions are small, which they are when no electric field is applied. The computed value of $\bar{\beta}$ may then be compared with the tilt angle measured from the actual conoscopic figure.

In the second simulation the method of calculating the optical transmittance described in section 2.8 is applied to the cell and crossed polarisers shown schematically in figure 4.5. The method divides up the LC layer into slices so thin that the variation in optical properties across each layer becomes negligible (approximately 100 slices per micron of cell thickness). A cubic spline is fitted to the ϕ and ψ values calculated in section 4.3 to evaluate the director orientation for a total of 720 slices across the $7 \mu m$ cell. From these values of ϕ and ψ the tilt and twist angles of the n-director, β and α , are calculated using equations 4.5 and 4.6. The cell rotation angle η is included in the optical method described in section 2.8 by adding the value of η onto each director twist angle. Table 4.1 gives the dimensions of the LC cell and table 4.2 gives the values of the optical constants used in the calculations. To find the apparent azimuthal angle, α_{app} , the cell rotation angle η is altered to minimise the transmitted intensity.

The principle underlying the second simulation is illustrated by placing a bire-

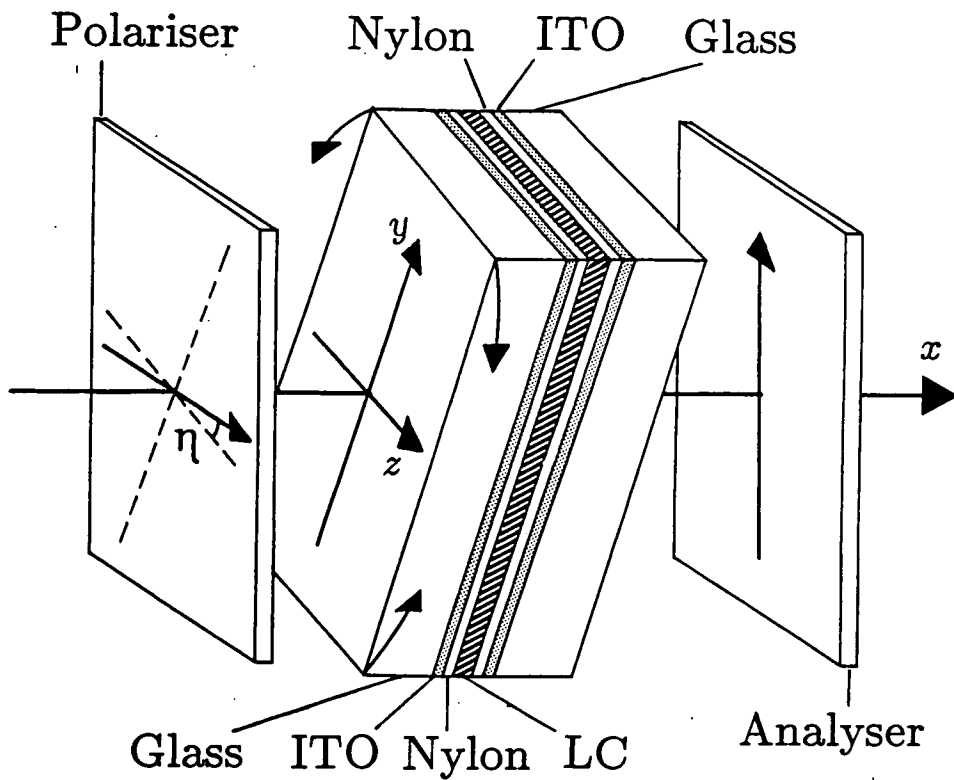


Figure 4.5: Model of the LC cell used in the optical calculations. The polariser and analyser are crossed and the LC cell is rotated about the x -axis to find the minimum transmission orientation. The rubbing direction is parallel to the z -axis and makes an angle η with the polariser axis.

Material	Thickness
Liquid crystal (B.D.H. SCE3)	$7 \mu m$
Nylon	$0.1 \mu m$
ITO	$0.05 \mu m$
Glass	1 mm

Table 4.1: Specification of the LC cell

fringing slab between crossed polarisers. The transmitted intensity is given by

$$I = I_o \sin^2(2\eta) \sin^2 \left[\frac{\pi(n_{eff} - n_o)d}{\lambda} \right] \quad (4.37)$$

where I_o is the incident intensity, η is the angle which the optic axis makes with the front polariser axis, d is the sample thickness, n_{eff} is the effective extraordinary refractive index (given by equation 4.36) and λ is the wavelength of the light in vacuo. The orientation of the projection of the optic axis onto the plane of the slab is found by rotating the slab until the minimum transmission orientation is found. The projection of the optic axis is then aligned with the polariser axis. In general in a LC the optic axis varies in orientation throughout the sample and may not waveguide the light. However the value of η which gives the minimum transmission, which we define to be the apparent azimuthal angle α_{app} , does yield an apparent value for the orientation of the optic axis, a parameter which may be readily measured.

In summary, simulations of the value of the average tilt angle $\bar{\beta}$ and the variation of apparent azimuthal angle α_{app} with applied voltage provide us with two experimentally verifiable predictions of the theory proposed in this chapter. Before looking in detail at the results of the simulations the experimental techniques used are described.

LC extraordinary refractive index, n_e	1.69
LC ordinary refractive index, n_o	1.50
Nylon refractive index, n_{nyl}	1.53
ITO refractive index, n_{ITO}	2.0
Glass refractive index, n_{gl}	1.54

Table 4.2: Optical constants used in the calculation

4.5 Experimental Measurements

4.5.1 Measuring the Apparent Azimuthal Angle

The construction of the LC cell used is shown schematically in figure 4.5. Each of the ITO-coated glass plates was spin-coated with nylon and rubbed unidirectionally with lens tissue wrapped around a 20 mm diameter cylinder. Short sections of 7 μm diameter glass fiber rod were spread randomly over the lower plate to space the plates a uniform distance apart with the rubbing directions parallel. The cells were supplied complete by S.T.C. Technology Limited. In all of the experiments described below the B.D.H. liquid crystal SCE3 was used. Table 4.3 lists some of the physical properties of this material which exhibits the following phase transitions at the temperatures shown:

$$-20^{\circ}\text{C} \xrightleftharpoons{SmC^*} 74^{\circ}\text{C} \xrightleftharpoons{SmA} 105^{\circ}\text{C} \xrightleftharpoons{N^*} 136^{\circ}\text{C} \xleftarrow{I}. \quad (4.38)$$

In relation 4.38 SmA denotes the smectic A phase, N^* denotes the chiral ne-

Spontaneous polarisation, P_s	$88\mu\text{Cm}^{-2}$
Cone angle, θ	25.5°
Parallel dielectric constant, $\epsilon_{\parallel}$	3.10
Perpendicular dielectric constant, $\epsilon_{\perp}$	5.04

Table 4.3: Specification of the B.D.H. LC SCE3 at 15°C

matic phase and I denotes the isotropic phase. To ensure good alignment the manufacturers have adjusted the nematic pitch so as to be as long as possible at the $SmA \leftrightarrow N^*$ phase transition temperature. The empty cell was first heated to above the nematic-isotropic transition temperature and was then filled by capillary action. After the cell had been allowed to cool to room temperature it was sealed with epoxy resin on all four sides. Uniform director alignment was

produced by heating the complete cell into the nematic phase and cooling it very slowly into the *SmA* phase and finally into the *SmC** phase. From a number of such cells one was selected which had an even optical texture and uniform birefringence colour over its entire surface area.

Figure 4.6 shows schematically the optical system used to measure the apparent azimuthal angle of the LC cell. A sodium discharge lamp was used as the light source because available refractive index data for SCE3 had been measured for the sodium D spectral lines. The collimator consisted of a condenser lens, a 1mm diameter pinhole and a collimating lens. An iris diaphragm was used to reduce the beam diameter to 3mm, and the light was passed through high quality sheet polarisers (Melles Griot) placed either side of the LC cell. Light transmitted through the system with the polaroids crossed was focussed onto a photodiode (RS7900) and the output was monitored by a digital voltmeter (Keithley 179 TRMS). A bipolar square-wave voltage was applied across the cell to avoid the electrolytic degradation which accompanies prolonged application of d.c. voltages. The amplitude of the signal could be set anywhere in the range

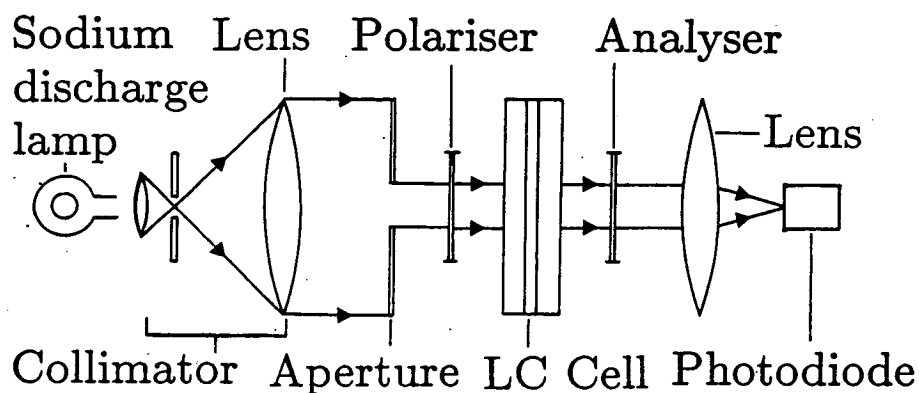


Figure 4.6: Schematic diagram of the optical system used to measure the apparent azimuthal angle of the LC cell.

0 – 20V by using a voltage divider and the frequency of the waveform was set to 0.1 Hz (cf the LC switching frequency of ~ 10 kHz) to permit measurement of

d.c. field effects on the optical properties of the cell. The LC cell was clamped into position on a rotatable mount which had a vernier scale calibrated to 0.1° .

Measurement of the apparent azimuthal angle for a particular voltage amplitude was made by noting the minimum transmission orientation for each voltage polarity. As far as could be seen these two orientations were symmetrically positioned on either side of the rubbing direction. The positions of the two minima were determined to within an absolute error of 0.5° and the apparent azimuthal angle was calculated by halving the angle between them. For voltages of 1V or less the measurements were made using d.c. voltages. To ensure that the whole cell was in a single state the voltage was initially set to $\sim 5\text{V}$ and reduced to the required value.

The apparatus described above was also used to check the cell thickness. First the cell was driven into one state and the voltage was reduced to zero. An optically uniform and defect-free texture indicated that the cell was in a single state. The minimum transmission orientation of the cell was located and a Babinet-Soleil compensator (Melles Griot) was inserted into the light beam behind the LC cell. The compensator was set to give a small retardation ($\sim 100\text{nm}$) and rotated until the minimum transmission orientation was found. To make sure that the extraordinary axes of the LC and compensator were perpendicular rather than parallel it was checked that the inclusion of the compensator produced a birefringence colour[76, chapter 9] equivalent to a smaller retardation than that of the LC alone. A retardation of $1.348\mu\text{m}$ was measured which, for a birefringence of 0.19, indicates a cell thickness of $7.1\mu\text{m}$ in good agreement with that expected. This was a rough check because it included the assumption that the LC waveguides the light and also that the n-director was always parallel to the cell walls.

4.5.2 Conoscopic Measurements

Conoscopic figures are usually observed by means of a polarising microscope – see chapter 3 and [72, chapter 4]. A parallel beam of light is passed through a polariser, a condensing lens, the sample, the objective lens and an analyser (which is crossed with respect to the polariser), emerging as a parallel beam. The conoscopic image is formed by the interference of the ordinary and extraordinary waves in the back focal plane of the objective lens. In a polarising microscope the Bertrand lens is inserted so that the ocular produces a viewable image of the conoscopic figure. When observed with white light the figure is described in terms of isochromes and isogyres. Isochromes are lines of equal colour and isogyres are parts of the figure where extinction occurs. Both isochromes and isogyres yield information about the orientation of the optic axis/axes of the medium. In particular for a uniaxial sample the pattern of the isogyres and the way in which this pattern moves when the sample is rotated provides information about the angle at which the optic axis is tilted with respect to the plane of section. A detailed description of the conoscopic technique is given in chapter 3.

Although SmC* LCs are slightly biaxial, to a good approximation they may be considered to be uniaxial [60] and their conososcopic figures may be interpreted accordingly. Chapter 3 describes the technique which we have developed to quantitatively interpret conoscopic figures. Figure 4.7 shows the conoscopic figure produced by the $7\mu\text{m}$ LC cell described in section 4.5.1. This conoscopic figure is shown in chapter 3 to be consistent with an average n-director tilt angle of $2 \pm 1^\circ$.

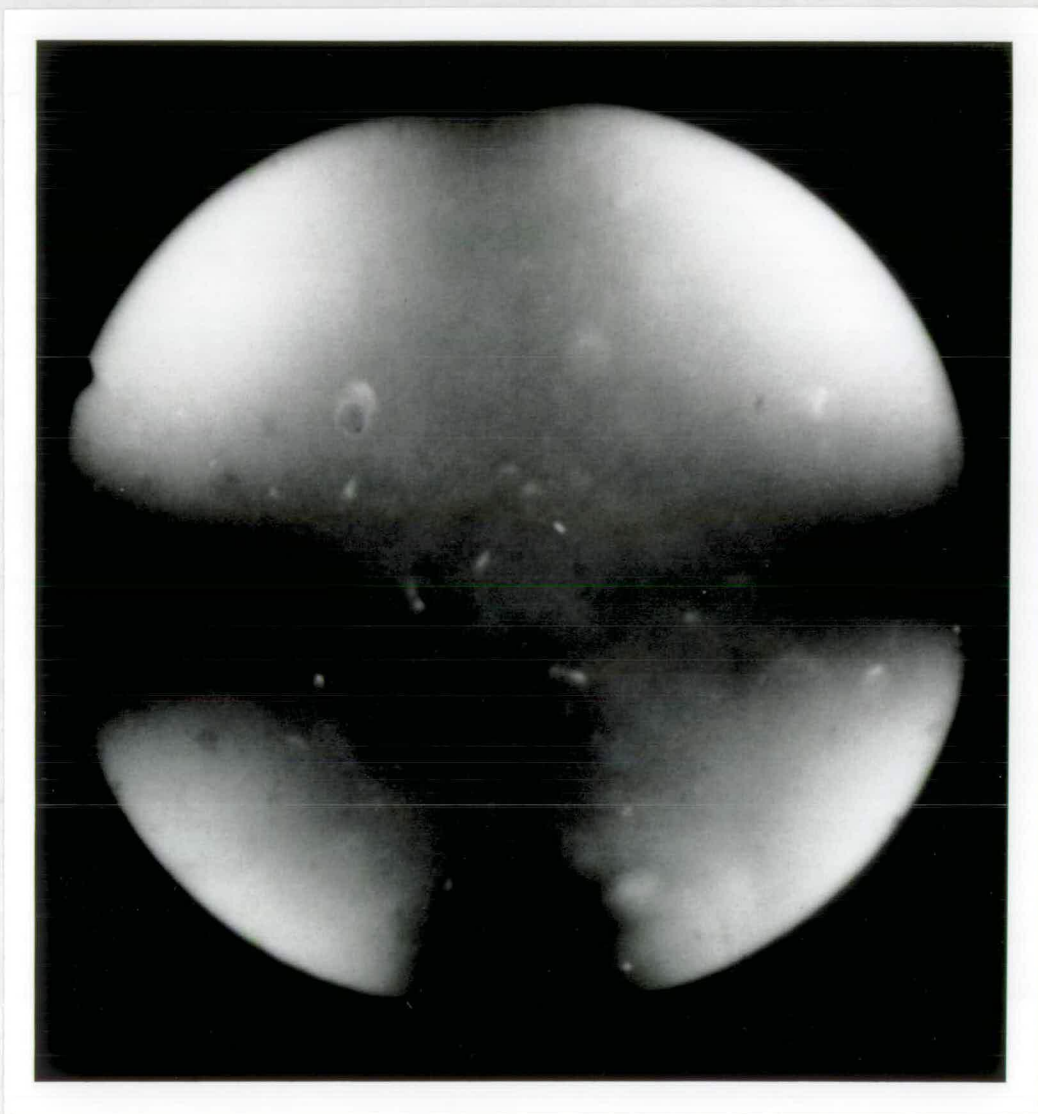


Figure 4.7: Conoscopic figure obtained for the LC SCE3 in a $7\mu\text{m}$ thick cell. The figure is consistent with an average n-director tilt angle of $2 \pm 1^\circ$.

4.5.3 Helical Pitch Measurement

In section 4.3.2 it was shown that the value of the chiral elastic constant D depends on the pitch of the helical structure occurring in a bulk sample of SmC* LC. If the LC is contained within a thick cell (say $100\text{ }\mu\text{m}$) then the surfaces produce homogeneous alignment of the n-director in their vicinity. However the surface interactions are insufficient to unwind the helix in the middle of the cell. These two structures are incompatible and lead to a regular distribution of linear defects as shown by Glogarova *et al.* [78]. These defects run parallel to the smectic layers and are clearly visible in both polarised and unpolarised light. Figure 4.8 shows these dechiralisation lines in a $100\text{ }\mu\text{m}$ cell containing the LC SCE3. The separation of these lines is precisely one helical pitch length and was measured by using a graticule to be $5.8\text{ }\mu\text{m}$ at 15° C . This value was subsequently used in the calculation of the value of the D constant.

4.6 Simulation Results and Comparison with Experimental Results

It was observed experimentally that the apparent azimuthal angle in a $7\text{ }\mu\text{m}$ cell containing SCE3 was 1.5° when no voltage was applied to the cell. The value of ϕ_0 was determined, subject to the assumptions made in section 4.2, by using equation 4.6. Then, using the data in tables 4.1 and 4.2 the theoretical model described in sections 4.2 to 4.4 was applied to a $7\text{ }\mu\text{m}$ cell to predict the ϕ and ψ configurations for different cell voltages. Figure 4.9 shows the predicted variations of ϕ and ψ through the cell. The effect of the chiral elastic energy is shown by the asymmetry (about the central plane of the LC) of the ϕ and ψ variations. Figure 4.9 also shows, for comparison, the predicted ϕ and ψ variations when no voltage is applied to the LC and the chiral elastic

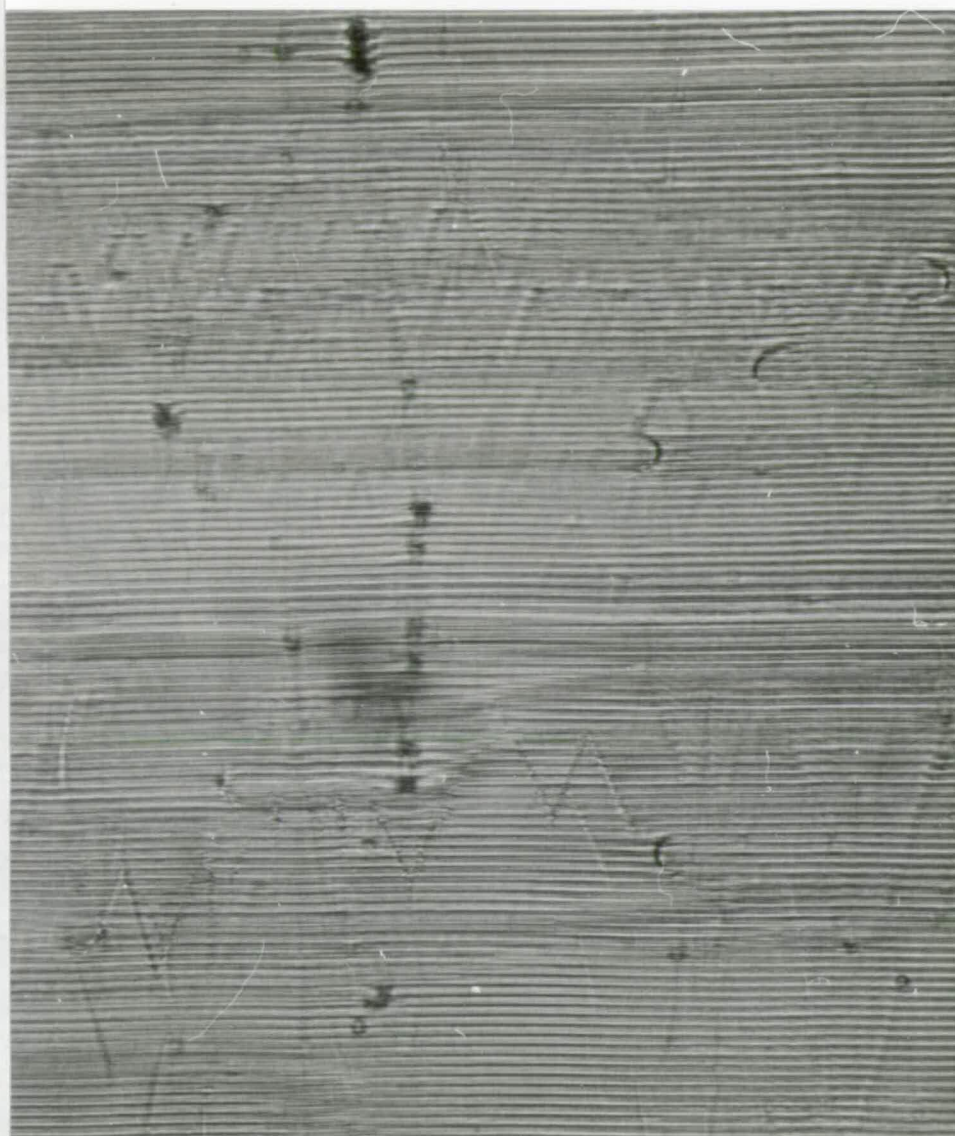


Figure 4.8: Dechiralisation lines exhibited by a $100\mu\text{m}$ thick LC cell containing SCE3 viewed in unpolarised light. These regularly spaced lines are linear discontinuities in the director orientation caused by the incompatibility of the orientations of the helical bulk director and the uniform surface director.

constants are set to zero. In all these calculations the following values were used: $B = 6 \times 10^{-12}$ N, $\sigma = 4.5 \times 10^{-5}$ N, $\phi_o = 86.5^\circ$ and $\gamma = 5$.

The variation in apparent azimuthal angle with voltage, calculated from the predicted values of ϕ and ψ , is shown in figure 4.10 along with the experimentally measured values. The correspondence between theory and experiment is seen to be excellent. In addition it was noted that the calculated mean tilt angle, $\bar{\beta}$, was 0.1° which agrees well with the conoscopic data.

The static properties of a SSFLC device are summarised in equation 4.37. Optimum contrast between the two stable states is obtained when the difference in orientation between the two states ($2\alpha_{app}$) is 45° and the effective birefringence is such that the device behaves as a half-wave plate. If a low birefringence LC is used in a thick cell then the performance of the device is less sensitive to absolute variations in thickness than a high birefringence LC in a thin cell. However the zero-field value of η is only 1.5° in a $7\mu m$ cell compared with a value of more than 10° in a $2\mu m$ cell. This effect is shown in chapter 5 to be related to the recently discovered chevron layer structure [67]. The contrast ratio between the two states is therefore much lower in thick cells than in thin cells, even when η is increased by a.c. stabilisation [79]. It is suggested therefore, that in applications requiring high contrast over relatively small areas, such as spatial light modulators, thin cells should still to be used, but that in large-area displays where contrast is less important, thicker cells might give better optical uniformity and appearance.

In summary, a model has been proposed to describe the optical properties of a SSFLC cell of a thickness approaching the maximum for which surface stabilisation is effective. The computed properties model the optical properties of real cells accurately. Clearly the model has the potential to describe the dynamic properties of SSFLC cells also, although this would require that realistic values of the bulk and surface viscosities, η_v and η_s , were used. The assumptions

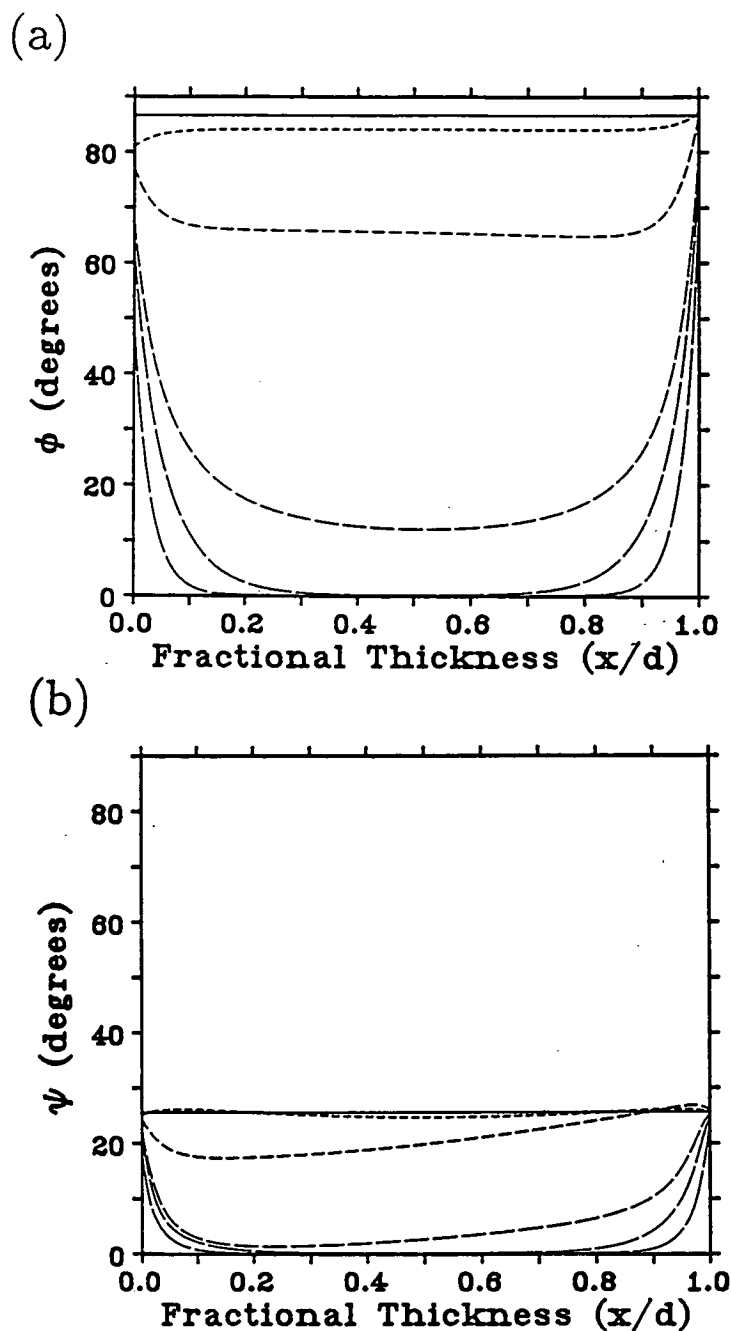


Figure 4.9: Computed variation of a) ϕ and b) ψ with fractional distance through the LC. The dotted curves and solid lines are the zero-voltage configurations with and without the chiral energy respectively. In order of increasing dash length the solid curves are the configurations including the chiral energy for applied voltages of 0.25V, 1V, 4V and 16V.

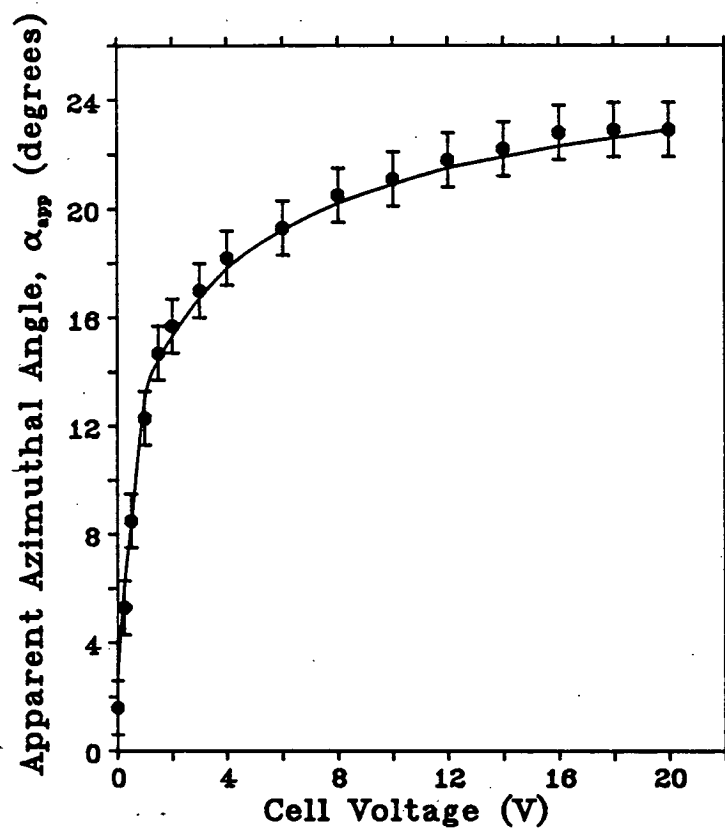


Figure 4.10: Variation of apparent azimuthal angle with cell voltage. The solid curve shows the computed points joined by a cubic spline and the points with the error bars represent the experimental measurements.

made in section 4.3.2 about the values of the elastic constants limit the model to a description of the elastic energy associated with c-director distortions and layer distortions. The coupling between the c-director distortions and layer distortions and the details of the relationships between the various chiral elastic constants are not considered.

In chapter 5 the rôle of the recently discovered chevron layer structure [67] in determining the director configuration is considered. A chevron layer structure is incorporated into the model described in this chapter and a physically based surface interaction potential is introduced in place of the one used in this chapter. The model based on the chevron layer structure is shown to provide a more complete description of the properties of SSFLC cells than the model described in this chapter.

4.7 Appendix A: Coefficients of the Minimum Free Energy Equation

The forms of the Γ_i in equations 4.26 and 4.28 are:

$$\begin{aligned}
 \Gamma_1 &= B_{13} \sin 2\psi \sin \phi - \cos^2 \psi (B_1 \sin^2 \phi + B_2 \cos^2 \phi) - B_3 \sin^2 \psi, \\
 \Gamma_2 &= \cos \psi \cos \phi (B_2 \sin \psi \sin \phi - C \cos \psi), \\
 \Gamma_3 &= \frac{1}{2} B_{13} \sin 2\psi \cos \phi - \frac{1}{2} (B_1 - B_2) \cos^2 \psi \sin 2\phi, \\
 \Gamma_4 &= \cos \psi \cos \phi [\cos \psi \sin \phi (B_2 - A \cos 2\phi) + C \sin \psi (3 \sin^2 \phi + 1)], \\
 \Gamma_5 &= \sin 2\psi (B_1 \sin^2 \phi + B_2 \cos^2 \phi - B_3) + 2B_{13} \cos 2\psi \sin \phi, \\
 \Gamma_6 &= -(D \cos \psi + D_1 \sin \psi \sin \phi + D_2 \cos \psi \cos 2\phi), \\
 \Gamma_7 &= -P_s E \cos \psi \sin \phi + \epsilon_o \epsilon_{\perp} E^2 e(\sin \psi \cos \theta - \cos \psi \sin \phi \sin \theta) \cos \psi \cos \phi \sin \theta, \\
 \Gamma_8 &= \Gamma_1, \\
 \Gamma_9 &= \Gamma_2, \\
 \Gamma_{10} &= D_1 \cos \psi \sin \phi - D \sin \psi, \\
 \Gamma_{11} &= -2\gamma \sigma_2 (\sin \beta \cos \psi \cos \phi \sin \theta) \exp[-\gamma \sin^2 \beta] + \\
 &\quad \begin{cases} \sigma_1 \gamma \sin \phi_1 \left(\frac{2\pi}{\pi+2\phi_o} \right) \exp[-\gamma \sin^2 \left(\frac{\phi_1}{2} \right)] & \text{if } \phi \notin [2m\pi + \phi_o, (2m+1)\pi - \phi_o] \\ \sigma_1 \left(\frac{\pi}{\pi+2\phi_o} \right) \sin 2\phi_2 & \text{otherwise.} \end{cases}
 \end{aligned}$$

The forms of the Λ_i in equations 4.27 and 4.29 are:

$$\begin{aligned}
 \Lambda_1 &= \frac{1}{2} C \sin 2\psi \sin 2\phi \cos \phi - B_2 \sin^2 \psi \sin^2 \phi - A \cos^2 \psi (1 - \sin^2 \phi \cos^2 \phi), \\
 \Lambda_2 &= \cos \psi \cos \phi (B_2 \sin \psi \sin \phi - C \cos \psi), \\
 \Lambda_3 &= \frac{1}{2} \sin 2\psi (B_3 - \sin^2 \phi (B_1 + B_2)) - B_{13} \cos 2\psi \sin \phi + C \cos^2 \psi \cos \phi, \\
 \Lambda_4 &= \frac{1}{2} A \sin 2\psi (1 - \sin^2 \phi \cos^2 \phi) - \frac{1}{2} B_2 \sin 2\psi \sin^2 \phi + \\
 &\quad C \sin \phi \cos^2 \phi (\cos^2 \psi - 2 \sin^2 \psi), \\
 \Lambda_5 &= \frac{1}{2} A \cos^2 \psi \sin 4\phi + C \sin 2\psi \cos \phi (\cos^2 \phi - 2 \sin^2 \phi) - B_2 \sin^2 \psi \sin 2\phi, \\
 \Lambda_6 &= D \cos \psi + D_1 \sin \psi \sin \phi + D_2 \cos \psi \cos 2\phi,
 \end{aligned}$$

$$\begin{aligned}
\Lambda_7 &= -P_s E \sin \psi \cos \phi + \\
&\quad \frac{1}{2} \epsilon_o \epsilon_{\perp} E^2 e [\sin 2\psi (\sin^2 \phi \sin^2 \theta - \cos^2 \theta) + \cos 2\psi \sin \phi \sin 2\theta], \\
\Lambda_8 &= \Lambda_1, \\
\Lambda_9 &= \Lambda_2, \\
\Lambda_{10} &= \frac{1}{2} D_2 \cos \psi \sin 2\phi, \\
\Lambda_{11} &= 2\gamma \sigma_2 \sin \beta (\cos \psi \cos \theta + \sin \psi \sin \phi \sin \theta) \exp(-\gamma \sin^2 \beta).
\end{aligned}$$

4.8 Appendix B: Solving the Minimum Free Energy Equations

This appendix describes the method developed by the author of solving the minimum free energy equations for a SmC* LC. The method is based on the fourth order Runge–Kutta (RK) method [70, page 277].

Consider an equation of the form

$$\frac{\partial \phi}{\partial t} = F(\phi, \psi, \Phi) \quad (4.39)$$

where $F(\phi, \psi, \Phi)$ is a known function of ϕ , ψ and Φ . Given the initial conditions that at $t = t_o$, $\phi(t = t_o) = \phi^o$, $\psi(t = t_o) = \psi^o$ and $\Phi(t = t_o) = \Phi^o$ the RK method allows the value of ϕ to be estimated a short time Δt later. The method states that provided Δt is not too large (see below) a good estimate of the value of ϕ at $t = t_o + \Delta t$ is

$$\phi(t = t_o + \Delta t) = \phi^o + [s_1 + 2(s_2 + s_3) + s_4]/6 \quad (4.40)$$

where

$$s_1 = \Delta t F(\phi^o, \psi^o, \Phi^o), \quad (4.41)$$

$$s_2 = \Delta t F(\phi^o + \frac{1}{2}s_1, \psi^o, \Phi^o), \quad (4.42)$$

$$s_3 = \Delta t F(\phi^o + \frac{1}{2}s_2, \psi^o, \Phi^o), \quad (4.43)$$

$$s_4 = \Delta t F(\phi^o + s_3, \psi^o, \Phi^o). \quad (4.44)$$

The RK method may be applied (with a change of variables) to any of the minimum free energy equations (4.26 to 4.29) or to the equation used to calculate the scalar potential (4.31). To calculate the values for the spatial derivatives in these equations the x-axis between $x = 0$ and $x = d$ is divided up into N intervals of length $\Delta x = d/N$. Each spatial derivative is approximated by the appropriate finite difference formula. If we define ϕ_{i-1} , ϕ_i and ϕ_{i+1} to be the

values of ϕ , at a particular time, at $x' = (i - 1)\Delta x$, $x = i\Delta x$ and $x = (i + 1)\Delta x$ respectively (not to be confused with $\phi_x = \partial\phi/\partial x$) then at that time

$$\phi_x = (\phi_{i+1} - \phi_{i-1})/2\Delta x, \quad (4.45)$$

$$\phi_{xx} = (\phi_{i+1} - 2\phi_i + \phi_{i-1})/(\Delta x)^2. \quad (4.46)$$

Similar formulae are used to calculate the spatial derivatives of ψ and Φ . At the edges of the LC layer ($i = 0, N$) the second derivatives of ϕ , ψ and Φ are never required but the first derivatives of ϕ and ψ are required. For $i = 0$ and N the finite difference approximations to ϕ_x are

$$\phi_x |_{i=0} = (\phi_1 - \phi_0)/\Delta x, \quad (4.47)$$

$$\phi_x |_{i=N} = (\phi_N - \phi_{N-1})/\Delta x. \quad (4.48)$$

Similar formulae are used to estimate the first derivative of ψ at the edges of the LC layer.

To calculate the director configurations through the LC layer two separate time systems are used: the first for the solution of equations 4.26 to 4.29 and the second for the solution of equation 4.31. Initial values of ϕ , ψ and Φ are specified and a value of N is chosen. Δt is calculated according to relation 4.32 and η_* is calculated according to relation 4.33. The values of ϕ and ψ are then calculated one time step forward in the first time system using the fourth order RK method four times, once each on equations 4.26 to 4.29. Taking the new set of values of ϕ and ψ the corresponding values of Φ are computed from equation 4.31 by iterating forward repeatedly in the second time system, using the RK method, until the values of Φ converge. The starting values of Φ for this iterative process are taken to be the values of Φ for the previous time step in the first time system. Once the values of ϕ , ψ and Φ are all known one time step forward in the first time system the whole process is repeated for further time steps until the values of ϕ and ψ converge at each point through the LC layer. This is the steady-state solution to the minimum free energy equations and describes the director orientation in the LC layer.

Chapter 5

The Chevron Layer Structure in SmC* LCs

5.1 The Chevron Layer Structure

In the previous chapter a model of SmC* LC cells was developed which is based on a tilted smectic layer. However Rieker *et al.* [67] have recently performed high-resolution x-ray scattering experiments on thin layers of SmC* LC which indicate that there are two well-defined SmC* layer orientations. The two layer orientations are present in equal amounts in a monodomain region of the LC and have equal and opposite layer tilt angles. Provided that the LC sample is prepared by cooling slowly from the nematic phase into the SmA phase they found that the layers in the SmA phase form perpendicular to the LC cell surfaces as shown in figure 5.1a. On cooling the LC into the SmC* phase they found that the symmetric chevron structure shown in figure 5.1b is formed and that the angle at which the layers tilt away from the surface normal, $\psi(T)$, increases as the temperature decreases. From measurements of the layer thicknesses in the SmA phase and the SmC* phase, d_A and $d_C(T)$ respectively, they found that

$$d_C(T) = d_A \cos \psi(T). \quad (5.1)$$

This relationship indicates that in the SmC* phase the smectic layers are effectively anchored to the alignment layers.

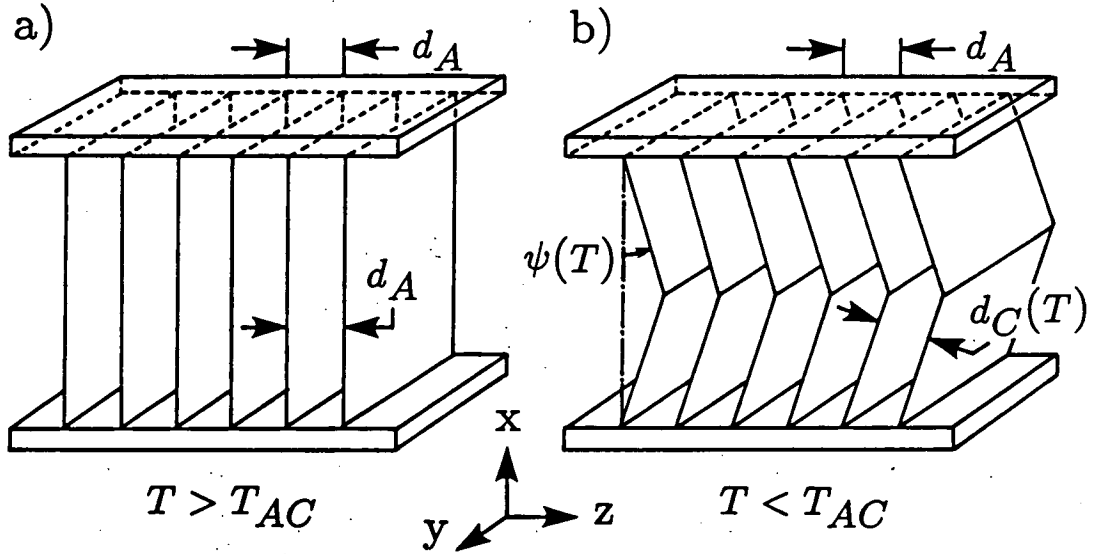


Figure 5.1: Schematic diagram of the smectic layer configuration in a) the *SmA* phase and b) the *SmC** phase. Above the *SmA*–*SmC** phase transition temperature, T_{AC} , the smectic layers are perpendicular to the LC surfaces. For temperatures below T_{AC} the smectic layers tilt at a temperature dependent angle, $\psi(T)$, away from the perpendicular. The smectic layer thickness in the *SmC** phase ($d_C(T)$) is related to the layer thickness in the *SmA* phase (d_A) and the layer tilt angle $\psi(T)$ by equation 5.1.

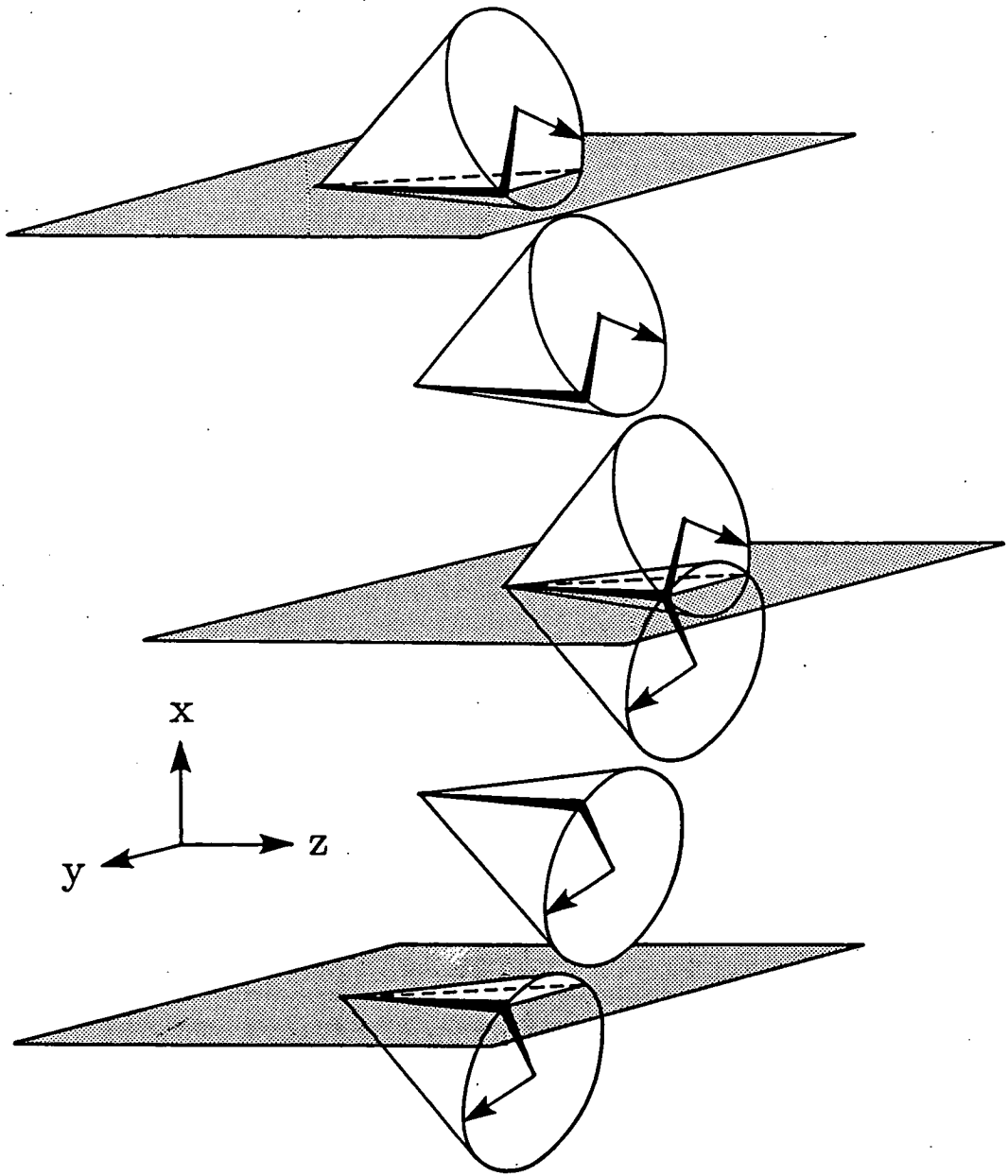


Figure 5.2: Schematic diagram of the uniform director configuration in a SmC^* LC cell with a symmetric chevron layer structure. The cones represent the loci of possible director configurations, the lines on the conical surfaces represent the $\mathbf{n}$ -director orientations and the arrows on the cone bases represent the orientation of the spontaneous polarisation $\mathbf{P}_s$. At every point through the LC the $\mathbf{n}$ -director is parallel to the LC surfaces and the plane of the chevron interface.

The simplest director configuration in a SmC* LC with a symmetric chevron layer structure is that shown in figure 5.2. At every point through the LC layer the n-director (the line marked on the conical surface of the cone) is parallel to the LC surfaces and the plane of the chevron interface and the spontaneous polarisation (represented by the arrows) is pointing slightly downwards. There are two stable states with a uniform director configuration: the state just described and shown in figure 5.2, and the state in which the n-director is parallel to the other intersection of the cones at the chevron interface, with the spontaneous polarisation pointing slightly upwards. Elston *et al.* [60] have shown, by looking at the optical resonance modes in a LC-filled Fabry-Perot cavity, that this uniform director structure can occur in SmC* LC cells. Their experiments also indicated that there is no more than 2° average n-director tilt angle within such a cell, that the chevron interface is confined to a region less than 100nm thick (which agrees with the x-ray measurements [67]) and that any boundary layers where there is rapid change of director orientation, if they exist, must be confined to regions which are less than 100nm thick. Extrapolating their measurements (which are given for temperatures from 20°C to 80°C) graphically the uniform twist angle, α , for the LC SCE3 at 15°C is found to be 14°. See figure 4.3 for definitions of the angles which describe the director orientation. Assuming that the n-director tilt angle, β , is zero throughout the LC layer as in figure 5.2 then the layer tilt angle ψ is found by rearranging equations 4.5 and 4.6 to give

$$\tan \psi = \pm \tan \theta \left(1 - \frac{\sin^2 \alpha}{\sin^2 \theta} \right)^{\frac{1}{2}}. \quad (5.2)$$

For a cone angle θ of 25.5° equation 5.2 gives values of ψ of $\pm 21.5^\circ$. Rieker *et al.* [67] found that the chevron layer tilt angle was independent of the surface treatment. We shall assume, on the basis of this observation, that a symmetric chevron occurs in our cells and that the layer tilt angles are $\pm 21.5^\circ$.

In the 7 μm thick SmC* LC cells which we have studied (see section 4.6) the apparent azimuthal angle (the angle between the extinction orientation and the

rubbing direction), α_{app} , was only 1.5° when no voltage was applied to the cell. The n-director orientation cannot therefore be uniformly parallel to the surface as in figure 5.2 or α_{app} would have a value of 14° . It is suggested in this chapter that the relaxed director structure is of the type shown in figure 5.3. In this configuration the twist angle of the n-director at the chevron interface is equal to 14° as in the uniform cell but the twist angle at the two surfaces is much less than 14° . Light normally incident on the LC, polarised parallel to the projection of the front-face director onto the LC surface, is waveguided (see section 2.1) along the director configuration, emerging polarised approximately parallel to the projection of the back-face director onto the LC surface. Therefore the value of α_{app} is approximately equal to the twist angle of the surface directors. In this chapter the elastic model presented in chapter 4 is extended to include a symmetric chevron layer structure in the relaxed (zero voltage) state. When the chevron layer structure is included in the model the complicated surface interaction energy density, f_{sur} , used in chapter 4 can be replaced by two simple terms which correspond directly to physical interactions. It is shown that the chevron model proposed explains well how the extinction orientation of the LC varies with voltage and is consistent with conoscopic measurements of the average n-director tilt angle.

5.2 A SmC* LC Model Including the Chevron Layer Structure

In this section the SmC* LC model developed in chapter 4 is modified to include a symmetric chevron layer structure. The n-director orientation at the chevron interface is assumed to be fixed, as a first approximation, parallel to the chevron interface and LC surfaces with a twist angle of 14° . Therefore the smectic layer orientations are fixed at the chevron interface: $\psi = -21.5^\circ$ in the limit as $x \rightarrow$

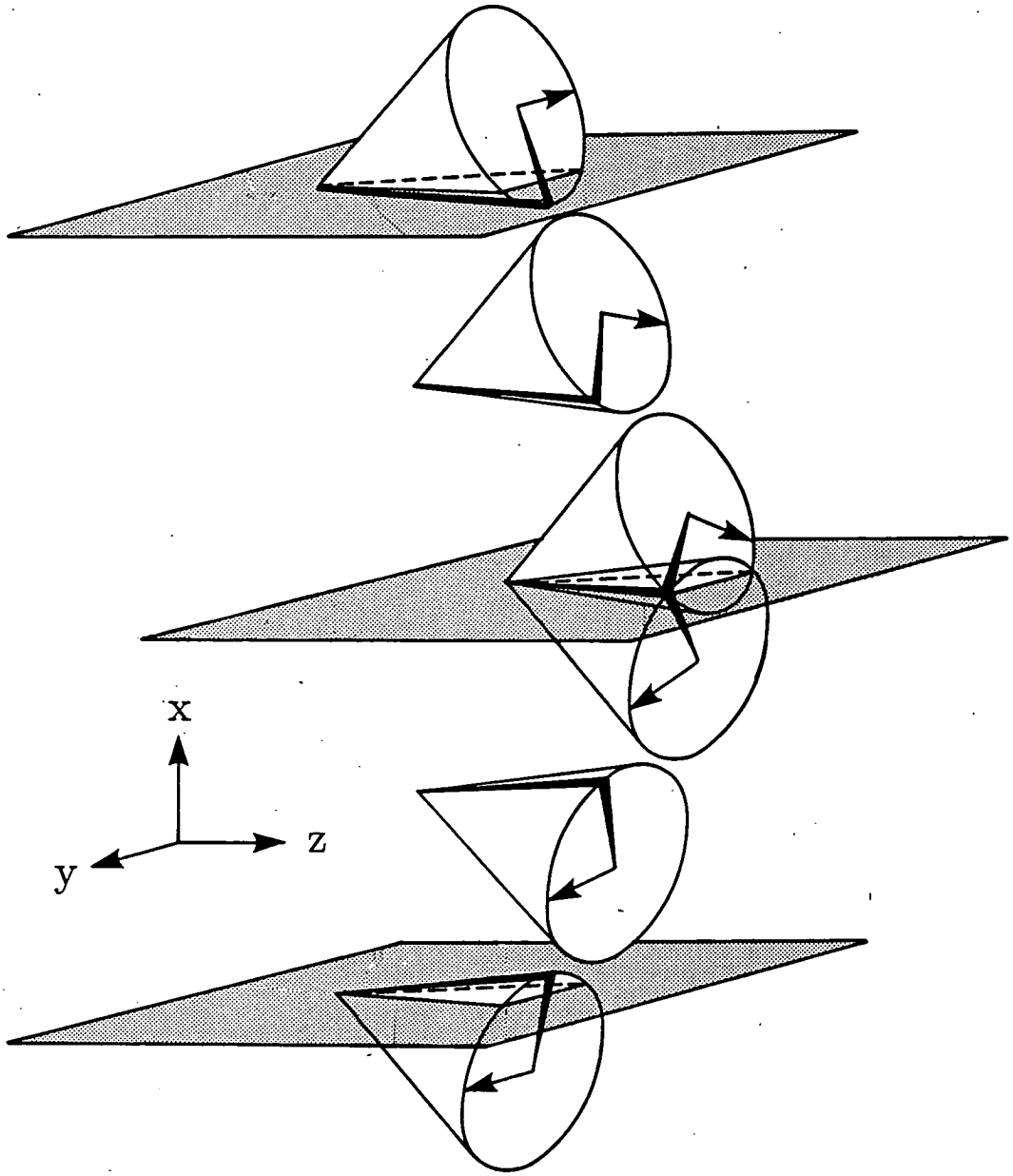


Figure 5.3: Director configuration proposed in this work. The layers are configured as a symmetric chevron in the relaxed (zero voltage) state and the director occupies one of the two positions defined by the intersections of the cones at the chevron interface. At the LC surfaces the alignment layer forces the $\mathbf{n}$ -director round until it is nearly parallel to the z -axis (rubbing direction).

$d/2$ from below and $\psi = 21.5^\circ$ as $x \rightarrow d/2$ from above. It is also assumed that the smectic layer orientations at the LC surfaces are fixed parallel to the layer orientations on the respective sides of the chevron interface. This restriction is applied so as to satisfy the anchoring condition, described in the previous section. As in chapter 4 we will neglect terms in the elastic free energy density, f_{elas} (equations 4.12 to 4.15), which describe the coupling between different elastic distortions, i.e. the terms in B_{13} , C_1 and C_2 , and consider only those terms which describe the elastic distortions themselves. If we neglect the chiral elastic energy terms, as a first approximation, and set the layer bend elastic constants A_{11} , A_{12} and A_{21} equal to A then, in terms of the angles ϕ and ψ , the elastic free energy density is

$$f_{elas} = \frac{1}{2}B_1(\phi_x \cos \psi \sin \phi)^2 + \frac{1}{2}B_2(\psi_x \sin \psi \sin \phi - \phi_x \cos \psi \cos \phi)^2 + \frac{1}{2}B_3(\phi_x \sin \psi)^2 + \frac{1}{2}A(\psi_x \cos \psi)^2 (\cos^2 \phi + \sin^4 \phi). \quad (5.3)$$

In this equation B_1 , B_2 and B_3 correspond to the bend, splay and twist distortions (see section 2.1) of the c-director and each subscript x denotes the operation $\partial/\partial x$. One final approximation is made in setting up this model: the dielectric anisotropy is assumed to have a negligible effect on the dielectric free energy density, f_d (equation 4.16), so that

$$f_d = -\frac{1}{2}\epsilon_o\epsilon_\perp \left(\frac{\partial \Phi}{\partial x} \right)^2 \quad (5.4)$$

where Φ is the electric scalar potential. Φ is related to the x-component of the electric field by $E_x = -\partial\Phi/\partial x$. This assumption will be valid provided that the n-director tilt angle is small ($< 5^\circ$). The free energy density associated with the interaction of the electric field with the spontaneous polarisation P_s , f_p , is given by equation 4.18. The total volume free energy density, f_{vol} , is given by

$$f_{vol} = f_{elas} + f_d + f_p. \quad (5.5)$$

With the introduction of the chevron layer structure the reason why there are two stable director configurations becomes clear: the two states correspond to

the two possible director orientations at the chevron interface. Therefore the complicated surface interaction energy density, f_{sur} , used in chapter 4 can be replaced by a much simpler function which describes directly the physical interactions taking place at the surfaces:

$$f_{sur} = -\sigma_{nem} \cos^2 \beta - \sigma_{al} \cos^2 \alpha. \quad (5.6)$$

In this expression the n-director tilt and twist angles, β and α , are given by equations 4.5 and 4.6. The first term in equation 5.6 describes a nematic type of surface interaction and has minimum energy when the n-director is parallel to the LC surfaces. The second term describes the alignment force produced by the rubbed nylon surface treatment and has minimum energy when the projection of the n-director onto the LC surface is parallel to the z-axis (rubbing direction).

To calculate the n-director orientation throughout the LC we minimise the volume and surface free energies with the respect to ϕ and ψ as described in section 4.3.1. The volume and surface torque balance equations are obtained by substituting the expressions for f_{vol} and f_{sur} given in equations 5.5 and 5.6 into equations 4.22 to 4.24. However equations 4.22 and 4.23 no longer apply at the midplane of the cell because the director orientation is fixed there. Equation 4.25 is redundant because ψ is fixed at the LC surfaces. With these substitutions we obtain the following simultaneous coupled partial differential equations:

$$\eta_v \frac{\partial \phi}{\partial t} = -(\Gamma_1 \phi_{xx} + \Gamma_2 \psi_{xx} + \Gamma_3 \phi_x^2 + \Gamma_4 \psi_x^2 + \Gamma_5 \psi_x \phi_x + \Gamma_7), \quad (5.7)$$

$$\eta_v \frac{\partial \psi}{\partial t} = -(\Lambda_1 \psi_{xx} + \Lambda_2 \phi_{xx} + \Lambda_3 \phi_x^2 + \Lambda_4 \psi_x^2 + \Lambda_5 \psi_x \phi_x + \Lambda_7), \quad (5.8)$$

$$\eta_s \frac{\partial \phi}{\partial t} = (\mathbf{x} \cdot \mathbf{s})(\Gamma_8 \phi_x + \Gamma_9 \psi_x) - \Gamma_{11}, \quad (5.9)$$

where the forms of the Γ_i and Λ_i are given in appendix A. In the above expressions η_v and η_s are volume and surface rotational viscosities, $\mathbf{x}$ is a unit vector parallel to the x-axis and $\mathbf{s}$ is the unit surface normal pointing into the LC at each surface. The solution of equations 5.7 to 5.9 depends on the strength of the electric field within the LC. If we minimise the volume free energy with respect

to Φ we find that

$$\epsilon_o \epsilon_{\perp} \frac{\partial^2 \Phi}{\partial x^2} = P_s (\psi_x \sin \psi \cos \phi + \phi_x \cos \psi \sin \phi) \quad (5.10)$$

which is the right hand side of equation 4.31. The solution to equation 5.10 for a particular set of values of ϕ and ψ determines the values of the scalar potential, and therefore the electric field strength, through the LC.

Equations 5.7 to 5.9 are solved by discretising the space and time coordinates into steps of length Δx and Δt respectively and using the fourth order Runge-Kutta method as described in sections 4.3 and 4.8. Since the chiral elastic constants have been set to zero the values of ϕ and ψ are antisymmetric about the chevron interface and it is only necessary to solve equations 5.7 to 5.9 for ϕ and ψ over the range $x \in [0, d/2]$. In the range $x \in [d/2, d]$, ϕ and ψ are given by the relationships

$$\phi(d - x_o) = -\phi(x_o), \quad (5.11)$$

$$\psi(d - x_o) = -\psi(x_o). \quad (5.12)$$

The starting configuration for ϕ in the range $x \in [0, d/2]$ is taken to be a linear variation from $\phi = -90^\circ$ at $x = 0$ to $\phi = -55.8^\circ$ (the value computed by setting $\beta = 0$ and solving equation 4.6 for ϕ) at $x = d/2$ and for ψ is taken to be a constant value of -21.5° . The antisymmetry of ϕ and ψ also makes the x-component of $\mathbf{P}_s$ symmetric about the chevron interface so that E_x is symmetric. If a voltage V is applied across the LC then

$$\Phi(d - x_o) = V - \Phi(x_o) \quad (5.13)$$

and in particular $\Phi(d/2) = V/2$. Therefore equation 5.10 need only be solved over the range $x \in [0, d/2]$ subject to the boundary conditions that $\Phi(0) = 0$ and $\Phi(d/2) = V/2$. For a given set of ϕ and ψ values equation 5.10 can be solved efficiently in the following way. First the equation is written in its finite difference form:

$$\epsilon_o \epsilon_{\perp} \left[\frac{\Phi_{i+1} - 2\Phi_i + \Phi_{i-1}}{(\Delta x)^2} \right] = P_s \left[\left(\frac{\psi_{i+1} - \psi_{i-1}}{2\Delta x} \right) \sin \psi_i \cos \phi_i + \left(\frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} \right) \cos \psi_i \sin \phi_i \right] \quad (5.14)$$

where each subscript refers to the x -coordinate of the variable i.e. Φ_{i+1} is the value of Φ at $x = (i + 1) \Delta x$. i runs from 0 at $x = 0$ to N at $x = d$. A finite difference equation in the form of equation 5.14 can be written down for each point along the x -axis between $x = 0$ and $x = d/2$ (not including the end points where the potential is already known). These equations are then written in the form of a tridiagonal matrix equation:

$$\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \vdots \\ \Phi_{N/2-2} \\ \Phi_{N/2-1} \end{pmatrix} = \begin{pmatrix} D_1 - \Phi_0 \\ D_2 \\ D_3 \\ \vdots \\ D_{N/2-2} \\ D_{N/2-1} - \Phi_{N/2} \end{pmatrix} \quad (5.15)$$

where D_i is the right hand side of equation 5.14 multiplied by $(\Delta x)^2 / \epsilon_o \epsilon_{\perp}$, $\Phi_0 = 0$ and $\Phi_{N/2} = V/2$. Finally equation 5.15 is solved for the vector $(\Phi_1, \Phi_2, \dots, \Phi_{N/2-1})^T$ using a library band-matrix solver (for example the NAG library routines F01LEF and F04LEF).

5.3 Simulation Results and Comparison with Experimental Results

The model described in section 5.2 generates a set of values of ϕ and ψ throughout the LC layer. Once a set of these values is known the optical method described in section 4.4 is applied to calculate the extinction orientation of a LC cell, with the computed values of ϕ and ψ , between crossed polarisers. Tables 4.1 and 4.2 list the values of the optical constants used in the calculations. The angle between the polariser axis and the rubbing direction when the LC

is in its extinction orientation defines the apparent azimuthal angle, α_{app} , for a particular voltage. In this section the computed values of ϕ and ψ produced by the chevron model are presented and a comparison is made between the predicted variation of α_{app} with voltage and the experimentally measured variation (see section 4.5.1).

To determine the values of the elastic constants in the SmC* LC chevron model a parameter survey is performed. At each stage of the parameter survey the computed values of α_{app} at voltages of 0V, 1V, 4V and 20V are compared with the experimentally measured values. The best match of the calculated and experimental values was obtained for $A = 4 \times 10^{-12} N$, $B_1 = 1 \times 10^{-12} N$, $B_2 = 4 \times 10^{-12} N$, $B_3 = 1 \times 10^{-12} N$, $\sigma_{nem} = 1 \times 10^{-4} N$ and $\sigma_{al} = 3 \times 10^{-5} N$. This indicates that, at least for this simple model, the c-director splay and layer bend elastic constants are dominant in the volume free energy and that, at the LC surfaces, the nematic energy term has a larger effect than the alignment energy term. For these values the ϕ , ψ , tilt and twist configurations computed are shown in figure 5.4. In addition to the previously noted symmetry of the ϕ and ψ configurations about the chevron interface the tilt angle configuration is antisymmetric and the twist angle configuration is symmetric. When no voltage is applied across the LC the twist angle configuration satisfies the condition for waveguiding (see section 2.1) so $\alpha_{app} \simeq \alpha(x = 0)$. Therefore the conoscopic figure (see chapter 3) produced by a LC cell with this director configuration will be very similar to the figure produced by a LC with a constant twist angle and the calculated tilt configuration. Actual conoscopic measurements indicate an n-director average tilt angle of $2 \pm 1^\circ$ which is in good agreement with the computed average n-director tilt angle of zero degrees.

To calculate the smectic layer shape from the values of ψ we introduce a function $g(x)$ which describes the layer's shape in the range $x \in [0, d]$. Values of $g(x)$ are

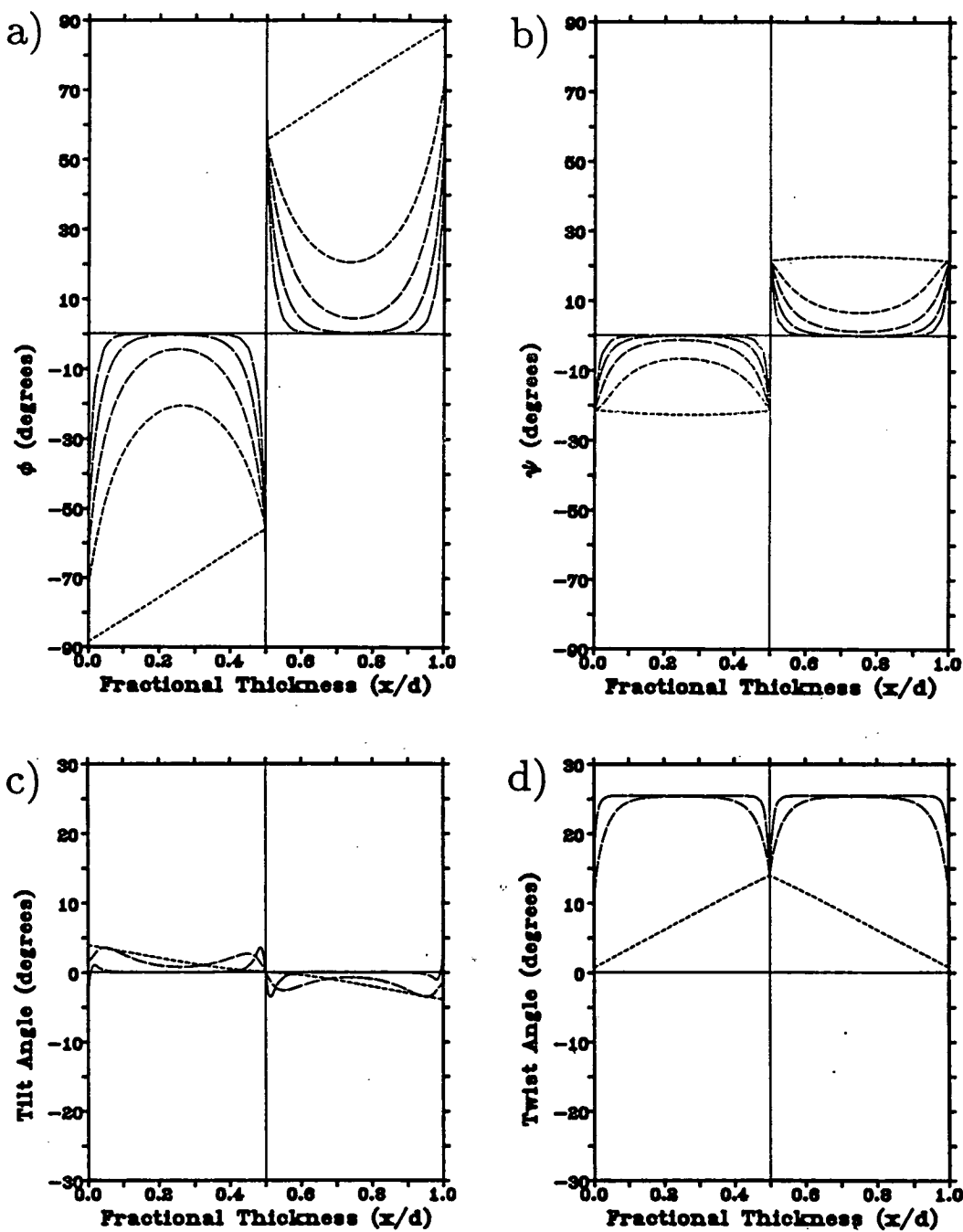


Figure 5.4: Computed variation of a) ϕ , b) ψ , c) tilt and d) twist with fractional distance through the $7\mu\text{m}$ thick LC cell. In a) and b) the curves are, in order of increasing dash length, for voltages of 0V, 0.25V, 1V, 4V and 16V. In c) and d) the curves are, in order of increasing dash length, for voltages of 0V, 1V and 16V.

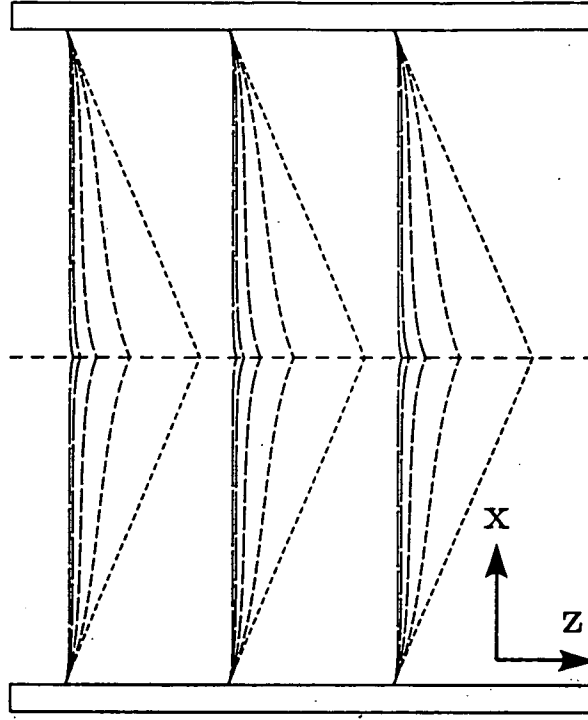


Figure 5.5: Calculated form of the smectic layers in a $7\mu\text{m}$ thick LC for various voltages. In order of increasing dash length the smectic layers are plotted for voltages of $0V$, $0.25V$, $1V$, $4V$ and $16V$.

computed using the relationship

$$\frac{dg(x)}{dx} = -\tan \psi(x). \quad (5.16)$$

Starting from $x = 0$ equation 5.16 is integrated numerically through the LC layer to $x = d/2$ using Euler's method. Values of $g(x)$ for $x \in [d/2, d]$ are found from relationship 5.12. Figure 5.5 shows the computed shape of the smectic layers. When no voltage is applied across the LC the layers form a symmetric chevron but they rapidly distort when a voltage is applied and tend, in the limit of large voltages, to a planar formation perpendicular to the LC surfaces.

Figure 5.6 shows the computed values and the experimentally measured values (see section 4.4) of the apparent azimuthal angle for different voltages. The

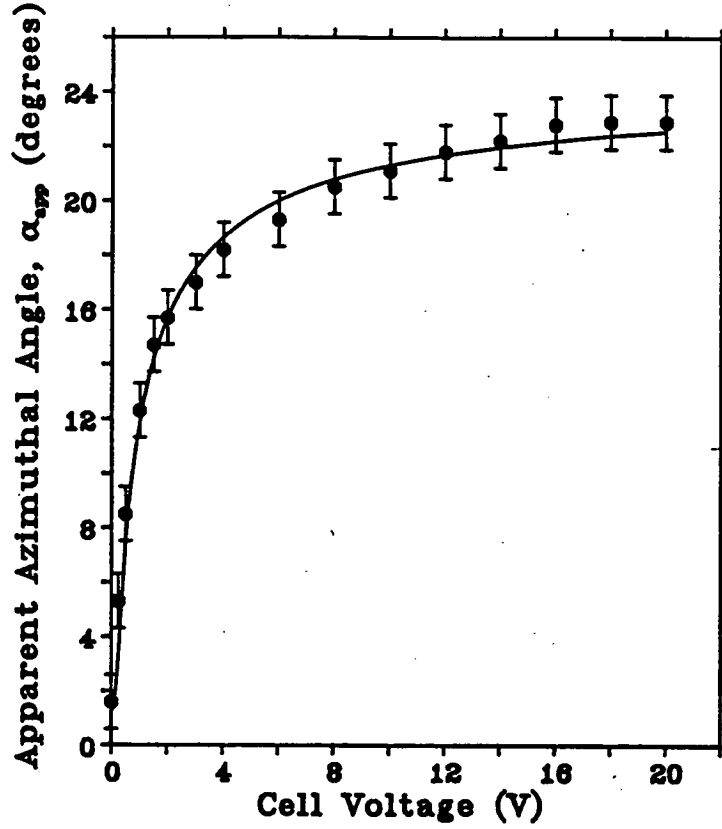


Figure 5.6: Variation of apparent azimuthal angle with LC cell voltage. The solid curve shows the computed points joined with a cubic spline and the points with the error bars represent the experimental measurements.

correspondence between theory and experiment is good.

In summary, a model has been presented based on the symmetric chevron layer structure. The model allows the smectic layers to bend when a voltage is applied to the LC. It is shown that the computed LC properties are in agreement with experimental conoscopic measurements of the relaxed director structure and with experimentally measured extinction orientations over a voltage range from 0 – 20V. Building the chevron layer structure into the model described in chapter 4 enables the complicated form of the surface interaction energy density to be replaced with a simple form directly related to the physical interactions at the surfaces. Finally, a relaxed director structure of the type shown in figure 5.3

suggests an explanation of why the value of α_{app} is larger for thin ($\sim 2\mu m$ thick) cells than for thick ($\sim 7\mu m$ thick) cells. In cells with identically prepared rubbed nylon LC alignment layers the values of α_{app} in the relaxed state were 1.5° and 8.5° for $7\mu m$ and $2\mu m$ thick cells respectively. As the cell thickness decreases and the (fixed) chevron interface director approaches the LC surface the surface director is increasingly twisted away from the rubbing direction. The increased surface director twist angle in thin cells produces the larger value of α_{app} observed in them. If the model described in this paper is used to calculate the relaxed director configuration in a $2\mu m$ thick cell then the computed value of α_{app} is 11° . The difference between this value and the measured value suggests that in thin cells the fixed chevron-director-orientation is not a good approximation and that the chevron director is pulled away from the orientation assumed here. It would be interesting to include a chevron interface free energy density in the director orientation calculations.

5.4 Appendix A: Coefficients of the Minimum Free Energy Equation

The forms of the Γ_i in equations 5.7 and 5.9 are:

$$\begin{aligned}
 \Gamma_1 &= -\cos^2 \psi (B_1 \sin^2 \phi + B_2 \cos^2 \phi) - B_3 \sin^2 \psi, \\
 \Gamma_2 &= B_2 \cos \psi \cos \phi \sin \psi \sin \phi, \\
 \Gamma_3 &= -\frac{1}{2}(B_1 - B_2) \cos^2 \psi \sin 2\phi, \\
 \Gamma_4 &= \cos^2 \psi \cos \phi \sin \phi (B_2 - A \cos 2\phi), \\
 \Gamma_5 &= \sin 2\psi (B_1 \sin^2 \phi + B_2 \cos^2 \phi - B_3), \\
 \Gamma_7 &= -P_s E \cos \psi \sin \phi, \\
 \Gamma_8 &= \Gamma_1, \\
 \Gamma_9 &= \Gamma_2, \\
 \Gamma_{11} &= -2\sigma_{nem} \sin \beta \cos \psi \cos \phi \sin \theta - \\
 &\quad 2\sigma_{ai} \sin \alpha \left(\frac{\sin \phi \sin \theta}{\cos \beta} + \frac{\cos^2 \phi \sin^2 \theta \cos \psi \sin \beta}{\cos^3 \beta} \right).
 \end{aligned}$$

The forms of the Λ_i in equation 5.8 are:

$$\begin{aligned}
 \Lambda_1 &= -B_2 \sin^2 \psi \sin^2 \phi - A \cos^2 \psi (1 - \sin^2 \phi \cos^2 \phi), \\
 \Lambda_2 &= B_2 \cos \psi \cos \phi \sin \psi \sin \phi, \\
 \Lambda_3 &= \frac{1}{2} \sin 2\psi [B_3 - \sin^2 \phi (B_1 + B_2)], \\
 \Lambda_4 &= \frac{1}{2} A \sin 2\psi (1 - \sin^2 \phi \cos^2 \phi) - \frac{1}{2} B_2 \sin 2\psi \sin^2 \phi, \\
 \Lambda_5 &= \frac{1}{2} A \cos^2 \psi \sin 4\phi - B_2 \sin^2 \psi \sin 2\phi, \\
 \Lambda_7 &= -P_s E \sin \psi \cos \phi.
 \end{aligned}$$

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Appendix A

Publications

The work presented in this thesis has also been described in the following papers:

1. A. R. MacGregor, "Modelling the Optical Properties of Twisted Nematic Guest-Host Liquid Crystals", J. Phys. D: Appl. Phys. **21**, 1438-1446 (1988);
2. A. R. MacGregor, "A Method for Computing the Optical Properties of a Smectic C* Liquid Crystal Cell", J. Opt. Soc. Am. A **6**, September 1989;
3. A. R. MacGregor, "A Method for Computing Homogeneous-Liquid-Crystal Conoscopic Figures", submitted to J. Opt. Soc. Am. A, June 1989;
4. A. R. MacGregor, "A Method for Computing the Optical Properties of a Smectic C* Liquid Crystal Cell with a Chevron Layer Structure", submitted to J. Mod. Opt., August 1989.

An early version of the first paper was presented, under the same title, at the 1988 British Liquid Crystal Society annual conference at Strathclyde University. Copies of each of the papers are given in the following pages.

Modelling the optical properties of twisted nematic guest–host liquid crystals

A R MacGregor

Department of Physics, University of Edinburgh, The King's Buildings,
Mayfield Road, Edinburgh EH9 3JZ, UK

Received 23 February 1988, in final form 16 May 1988

Abstract. Equations describing the deformation of a twisted nematic liquid crystal in an electric field in terms of the local mean molecular orientation (director) have been derived by Deuling. In addition Berreman has developed a method of describing the optical properties of such a cell. In this paper their model has been extended to take account of the degree of orientational disorder of the liquid crystal molecules. An electrical equivalent circuit of the cell is then introduced along with a method of computing the liquid crystal capacitance so that the fraction of the cell voltage appearing across the liquid crystal may be computed. Finally a comparison is made between the experimentally measured light transmission and that predicted by the theory with and without the molecular disorder correction. The overall agreement between theory and experiment is improved considerably when the molecular disorder correction is included.

1. Introduction

Nematic liquid crystals (LCs), including nematic guest–host LCs, are characterised by orientational order and positional disorder of their molecules. The director, a unit vector $\mathbf{n}$, is defined as the local mean molecular orientation. This direction coincides with the major axis of the dielectric ellipsoid and the optic axis defining the material's birefringent properties. In a guest–host LC a small quantity of dichroic dye (guest) with the properties shown in figure 1, is dissolved in a nematic LC (host). The dye is chosen so that its maximum absorption axis aligns parallel to the director and so that the visco-elastic and dielectric properties of the nematic host are virtually unchanged.

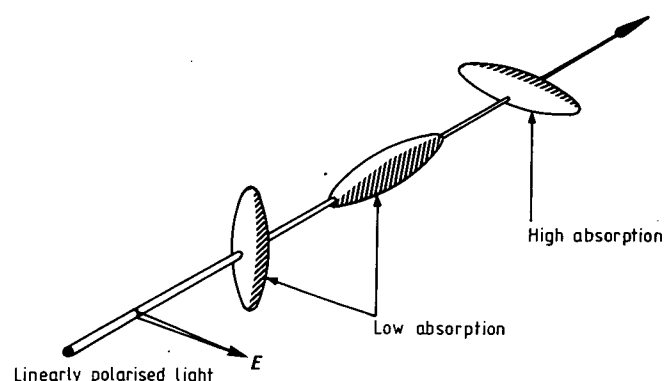


Figure 1. Light absorption by a dichroic dye molecule.

In a twisted nematic LC cell the dielectric and optical anisotropies are used to modulate light passing through the cell. Figure 2 shows schematically the construction of a typical LC cell and the specification of the one used is given in table 1. The transparent conducting layers of indium tin oxide (ITO) allow a voltage to be applied across the LC layer. Magnesium fluoride was evaporated obliquely onto the cell walls at an angle of thirty degrees to the surface-normal to a thickness of 120 ± 10 nm. Polyester sheet was used as a spacer between the cell walls and the cell was assembled in a laminar flow clean cabinet using a Perspex jig to ensure precise alignment. Epoxy resin was used to bond the cell which was then filled by capillary action with Roche LC mixture 1263. The cell was assembled so that the director orientations at the front and back planes were orthogonal.

The structure of the magnesium fluoride layers aligns the LC molecules near the cell walls producing the twisted director configuration shown in figure 3(a). By heating the LC cell to just above the nematic–isotropic transition temperature and then allowing it to cool slowly the twisted configuration was produced uniformly over the whole cell. Above a threshold voltage U_T , applied across the ITO electrodes, the director configuration distorts in the manner shown in figure 3(b).

Below the threshold voltage, linearly polarised light launched into the cell polarised parallel to the front-face director is waveguided along the uniformly twisted structure and is strongly absorbed by the guest dye

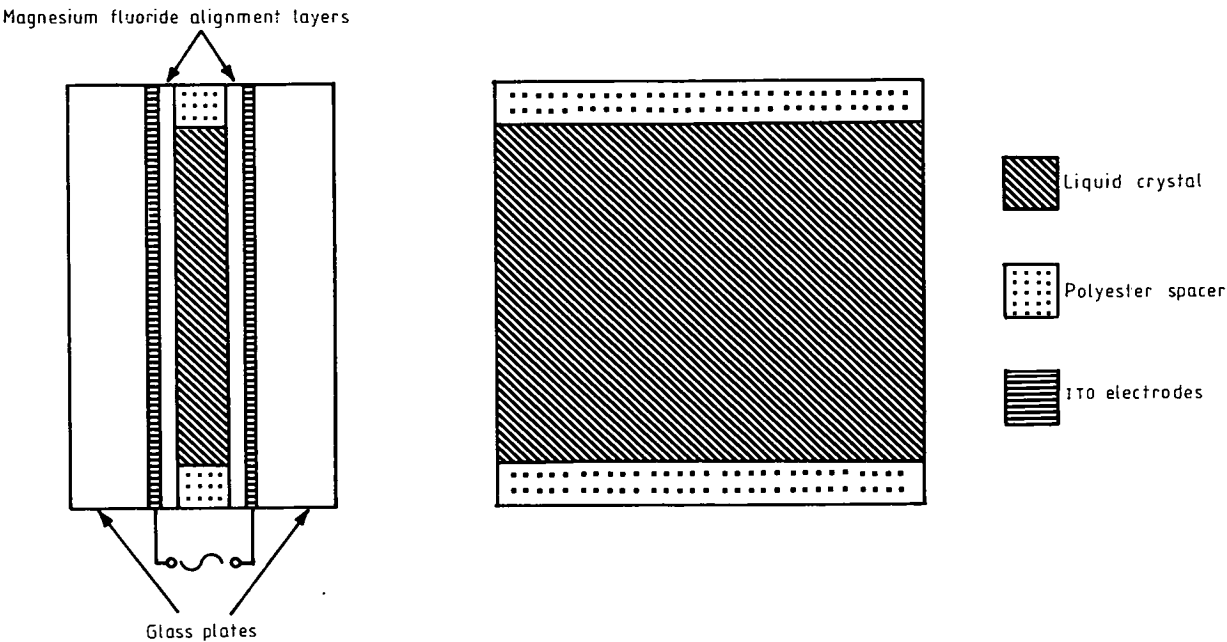


Figure 2. A schematic diagram of the LC cell (section and plan views).

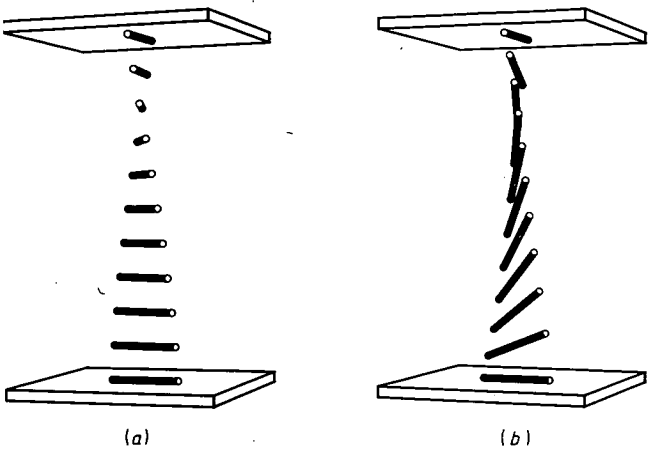


Figure 3. Twisted nematic director configuration with applied voltage $U \leq U_T$ (a) and $U = 2U_T$ (b).

molecules. However, for voltages above the threshold, the molecules tilt so they are no longer parallel to the cell walls. Light transmission then increases as the waveguiding breaks down and the absorption by the dye molecules decreases as they also tilt out of the plane.

The LC configuration described above was employed in a reflection-mode electronically addressed LC spatial light modulator [1] which has been used as a Fourier-plane filter in a coherent optical processing system. The reason for using a twisted instead of an untwisted cell is the sharper threshold observed for the transmission against voltage curve for the twisted cell [2].

In previous work on the optical properties of twisted nematics [3, 4] the LC molecules were all assumed to lie parallel to the director. However it is well known that nematic LCs scatter light strongly because of local orientational fluctuations. By taking this effect into account using a molecular disorder correction the agreement between theory and experiment is significantly improved.

2. Calculating the minimum-energy director configuration

Frank [5] has shown that an arbitrary elastic deformation of a nematic LC may be uniquely described as a linear combination of splay, twist and bend distortions. These distortions have associated elastic con-

Table 1. Specification of the LC cell.

Material	Thickness (μm)	Area (mm^2)	Dielectric constant
Glass	3.0×10^3	25×25	—
Indium tin oxide	0.05^a	25×25	—
Magnesium fluoride	0.12^b	25×25	1.912
Polyester spacer	13^c	2.5×25	3.8
LC layer thickness	13	20×25	—

^a Reference [4].
^b Measured using Talystep.
^c Measured using a digital micrometer.

stands k_{11} , k_{22} and k_{33} . For a cell of thickness L subject to electric field E at constant temperature and pressure the Gibbs' free energy associated with unit area of the cell is given by

$$G = \frac{1}{2} \int_0^L [k_{11}(\nabla \cdot \mathbf{n})^2 + k_{22}(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + k_{33}(\mathbf{n} \times \nabla \times \mathbf{n})^2 - \mathbf{D} \cdot \mathbf{E}] dz. \tag{1}$$

Equation (1) is valid for sinusoidal electric fields provided that the RMS field amplitude is used and that the field frequency is very much greater than the LC switching frequency.

The minimum-energy director configuration is found by minimising the right-hand side of equation (1) using the calculus of variations. However the equations derived by Deuling [3] are difficult to solve numerically at voltages above about 4 V RMS because they have an infinite singularity in them corresponding to the situation where the molecules in the centre of the cell are perpendicular to the cell walls. Welford and Sambles [6] have found an elegant solution to a similar problem in the equations describing planar (untwisted) nematic cells which avoids this problem by using a change of variables. Using the same substitution here to improve the behaviour of the numerical solution, thereby extending the voltage range over which solutions may be evaluated, the director configuration was calculated for voltages up to 7 V RMS for the LC specification given in table 2. The director orientation is described in terms of the tilt (θ) and twist (φ) angles defined in figure 4. Figure 5 shows the tilt and twist configurations across the cell for various values of the RMS voltage.

Of particular interest is the 1.74 V twist curve which is altered from the threshold voltage twist curve in the opposite sense to the twist change at larger voltages. This 'reverse twist' effect is important because it influences the optical transmission at low voltages. While the distortion threshold voltage is 1.46 V the apparent optical threshold occurs at voltages at least 0.5 V above this. The reason for the reverse twist can be seen by considering, in the following simple model, the way in which the distortion energy is partitioned between splay, twist and bend deformations.

As may be seen from the curves in figure 5 at the threshold voltage the twist angle $\varphi(z/L)$ varies linearly with the fractional distance z/L through the cell. At voltages just above threshold the twist angle deviates from this linear relationship and we assume that the twist angle may be approximated by the expression

$$\varphi\left(\frac{z}{L}\right) = \frac{\pi}{2}\left(\frac{z}{L}\right) - A \sin\left(\frac{2\pi z}{L}\right) \tag{2}$$

Table 2. Specification of the Roche LC mixture 1263.

Spray elastic constant, k_{11}	14.4×10^{-12} N
Twist elastic constant, k_{22}	7.0×10^{-12} N
Bend elastic constant, k_{33}	20.0×10^{-12} N
Parallel dielectric constant, $\epsilon_{ }$	12.3
Perpendicular dielectric constant, $\epsilon_{\perp}$	3.8

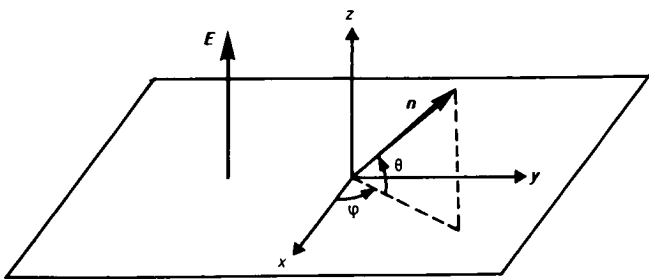


Figure 4. Definition of tilt and twist angles.

where A is the amplitude of the distortion. A positive value of A corresponds to the sense of twist at large voltages and a negative value of A to reverse twist. The tilt angle was taken as having the actual functional dependence given by the solution to the minimum free energy equations. In terms of the tilt and twist angles

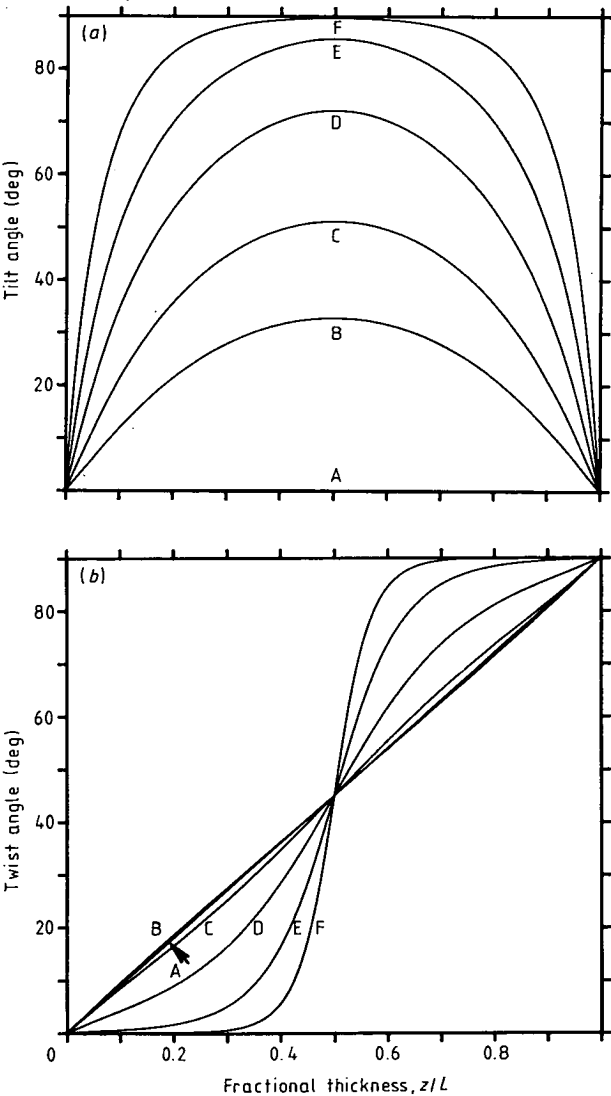


Figure 5. (a) Tilt (θ) and twist (φ) angles versus fractional distance through the LC cell with applied voltage $U = U_T = 1.46$ V (A), $U = 1.74$ V (B), $U = 2.09$ V (C), $U = 2.78$ V (D), $U = 4.17$ V (E) and $U = 6.95$ V (F).

Table 3. Twist and bend energies (arbitrary units) for different distortion amplitudes

A (deg)	Twist energy	Bend energy	Summed energy
-1	6.308	4.199	10.507
0	6.145	4.364	10.509
1	6.013	4.543	10.556

the Gibbs' free energy equation (1) is

$$G = \frac{1}{2} \int_0^L \left[(k_{11} \cos^2 \theta + k_{33} \sin^2 \theta) \left(\frac{\partial \theta}{\partial Z} \right)^2 + (k_{22} \cos^2 \theta + k_{33} \sin^2 \theta) \cos^2 \theta \left(\frac{\partial \varphi}{\partial Z} \right)^2 \right] dz - \frac{1}{2} \left(\frac{D_z^2}{\epsilon_0} \right) \int_0^L (\epsilon_{11} \sin^2 \theta + \epsilon_{\perp} \cos^2 \theta)^{-1} dz. \quad (3)$$

Only the third and fourth terms in equation (3), corresponding to twist and bend energies respectively, are functions of twist angle and therefore vary with A . These twist and bend energies and their sum were computed for various values of A at a voltage of 1.74 V between the distortion and optical threshold voltages. Table 3 lists these energies in arbitrary units.

Although the twist energy is higher for the reverse-twist configuration the bend energy is lower and by a greater amount. As the voltage is increased the energy minimum occurs for positive values of A corresponding to twist in the familiar sense.

3. LC cell optical properties

The optical properties of the LC cell are uniquely determined by the solution of Maxwell's equations. Berreman [7] showed how the transmitted and reflected electromagnetic fields may be calculated for an anisotropic medium using a 4×4 propagation matrix operating on a 4-vector which specifies the transverse electromagnetic field incident on the LC layer. Montgomery [8] extended the method to take account of the isotropic layers in the cell. In practice the solution may be calculated very accurately by careful implementation on a computer. It is found that an efficient way to do this is to divide the LC layer up into slices, approximating the variation in optical properties across each slice by a polynomial fitted to the data using Newton's divided difference formulae. A propagation matrix is then computed for each slice and the matrices are multiplied together to compute the propagation matrix for the whole LC layer. This is more efficient than treating the LC as a single thick slice because the elements of the propagation matrix are power series expansions which converge more rapidly for thin slices than for thick slices. However, the reduction in computation time for thin slices must be balanced against the increase in computation time due to the increased number of slices. Using 1000 slices provides such a balance.

Table 4. Optical constants and cell parameters used in computation.

LC extraordinary refractive index, n_e	1.639
LC ordinary refractive index, n_o	1.500
LC parallel absorption coefficient, $D_{\parallel}$	$0.3940 \mu\text{m}^{-1}$
LC perpendicular absorption coefficient, $D_{\perp}$	$0.0386 \mu\text{m}^{-1}$
Magnesium fluoride refractive index	1.383
ITO refractive index	2.0
Glass refractive index	1.54

In order to describe the optical properties of guest-host liquid crystals it is necessary to take account of the absorption caused by the dichroic dye. A simple way of doing this is to write Maxwell's equations using complex refractive indices whose imaginary components are directly proportional to the absorption coefficients [9]. Berreman's derivation may then be followed using the complex version of Maxwell's equations. The form of the solution only differs from the non-absorbing case in the replacement of the real refractive indices by complex ones.

Propagation matrices for the cover-glass, ITO and magnesium fluoride layers are also computed. These matrices are multiplied together, along with the LC layer propagation matrix, so that they operate on the vector describing the incident light wave in the same order that the light traverses the cell layers.

Reflected and transmitted electromagnetic fields are computed from the resulting vector. Table 4 lists the values of the optical constants used in the calculations.

If the degree of the polynomial used to fit the variation in optical properties from slice to slice is varied it is found that Scheffer's [2] approximation of uniform properties within slices incurs negligible errors. With this approximation the general form of the slice propagation matrix was multiplied out and used in all subsequent calculations, improving the speed of operation roughly fourfold.

4. LC cell electrical properties

We shall now determine the relationship between the cell voltage and the voltage applied to the LC layer, using the equivalent circuit shown in figure 6.

The resistance values required for figure 6 were measured directly and the capacitances of the spacers and the magnesium fluoride layers were calculated for a 1.6 kHz sinusoidal voltage signal from their dimensions and dielectric properties.

Using the tilt angle data the capacitance C_{LC} of the LC layer was calculated using

$$\frac{1}{C_{LC}} = \sum_{i=1}^{1000} \frac{1}{C_i}$$

where

$$\frac{1}{C_i} = \int_{z_{i-1}}^{z_i} \frac{dz}{\epsilon_0 \epsilon(\theta) A_{LC}} \quad (4)$$

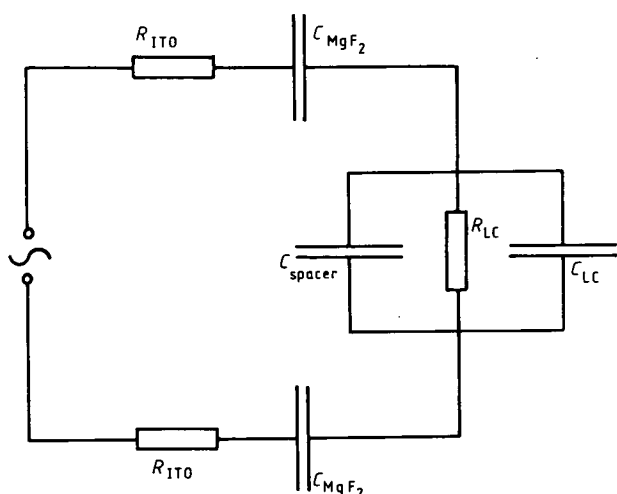


Figure 6. LC cell equivalent circuit. $R_{ITO} = 400 \Omega$, $C_{MgF_2} = 0.17 \mu F$, $C_{spacer} = 0.32 nF$, $R_{LC} = 2 M\Omega$.

where C_i is the capacitance of the slice i of thickness $Z_i - Z_{i-1}$ and area A_{LC} . The dielectric function $\epsilon(\theta)$ [10] is given by

$$\epsilon(\theta) = \epsilon_{\perp} \cos^2 \theta + \epsilon_{\parallel} \sin^2 \theta. \quad (5)$$

The integral in equation (4) was evaluated for each slice of the LC by fitting a polynomial of degree n to the tilt angle data for that layer and its neighbours. As in the optical calculation, negligible error was found to be introduced by assuming that the dielectric properties of the layer were uniform across it. Figure 7 shows the computed capacitance for a $13 \mu m$ cell.

With these values substituted into the equivalent circuit, the voltage dropped across the LC could be calculated for a variety of cell voltages, and these voltage values were used to provide curves showing the LC transmission versus applied cell voltage. The fraction of the cell voltage appearing across the LC layer varied slowly from 0.964 at threshold to 0.917 at the maximum voltage.

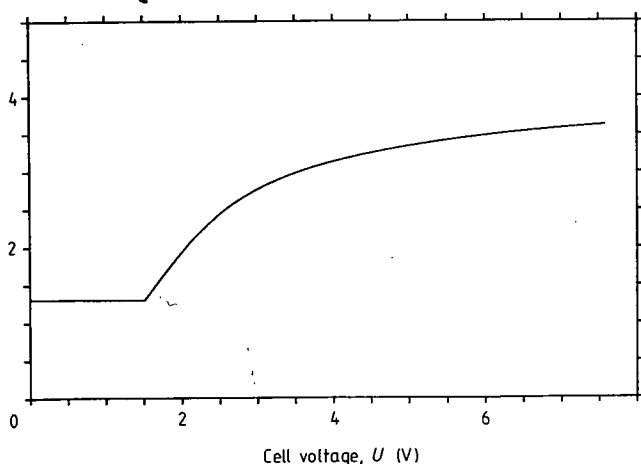


Figure 7. Computed capacitance of a $13 \mu m$ cell.

5. Molecular disorder and LC properties

5.1. Theory

In the preceding discussion the LC molecules were assumed to be perfectly ordered about the director. However the director specifies only the local mean molecular orientation and indicates nothing about the degree of orientational order. The order parameter S is a measure of this ordering and is defined by de Gennes (see p 24 in [11]) as

$$S = \frac{3}{2} \langle \cos^2 \alpha_1 \rangle - \frac{1}{2} \quad (6)$$

where α_1 is the local angle of deviation from the director and the angle brackets denote the average of the function. Separate order parameters for the host nematic and guest dye may be defined. However, in the following, as no detailed information was available from the manufacturer, the guest was assumed to be isomorphic with the host and the order parameters equal. For the Roche guest-host LC mixture 1263 at $22^\circ C$, $S = 0.77$. It is important to consider the effects of molecular disorder because of the non-linear relationship between molecular orientation and macroscopic optical and dielectric properties. It has been shown (see § 5.4 in [11]) that the frequency of the perturbations is of order MHz to GHz so the 1.6 kHz voltage signal will not resolve the orientational changes while they will be apparent to the $\sim 10^5$ GHz light signal. Therefore the mean values of the dielectric constants may be used correctly in the director and capacitance calculations. However, in the optical calculations, the local fluctuations in director orientation, resulting from the molecular disorder, must be taken into account. The observed transmission of a LC is measured on a timescale much greater than that of the director fluctuations. Therefore the theoretical transmission should be calculated by taking the mean of the value of the transmission evaluated for all possible variations in the director configuration correctly weighted by a probability density function in orientation. To do this it is necessary to know the values the complex refractive indices would have if the LC were perfectly ordered and also the probability density function in orientation.

Various models, summarised in [12], have been put forward to describe the local molecular probability density function in orientation $P_1(\alpha_1)$ based on the different molecular interactions, both attractive and repulsive. Saupe and Maier [13] have derived a form for $P_1(\alpha_1)$ based on a simplified model neglecting the steric repulsion forces. Since the slices considered in the optical calculation are only of order ten molecules thick the local director probability density function in orientation was assumed, in accord with [13], to have the form

$$P_1(\alpha_1) = \frac{\exp(\sigma \cos^2 \alpha_1)}{4\pi Z_\sigma} \quad (7)$$

where

$$Z_\sigma = \int_0^1 \exp(\sigma x^2) dx.$$

Here σ is a parameter which may be adjusted to vary the distribution width to take account of the difference between the theoretical situations considered. This function was used to describe the orientational ordering in each of the thousand slices of the optical calculation. In practice the value of σ is unknown so the relationship between the measured and perfectly ordered local refractive indices is also unknown. However, the values of the perfectly ordered refractive indices may be estimated using a global probability density function in orientation as shown below.

Light traversing the LC follows a path much longer than the coherence length of the fluctuations. Therefore, regardless of the form of the local probability density function in orientation, the time variation of the spatial average fluctuation, α , for the path will be approximately Gaussian in form. This result follows from the central limit theorem. On this basis we define a global probability density function in orientation $p_g(\alpha)$ which describes the fluctuations of α :

$$p_g(\alpha) = \frac{\exp(-\alpha^2/\omega^2)}{4\pi Z_\omega} \quad (8)$$

where

$$Z_\omega = \int_0^{\pi/2} \exp(-\alpha^2/\omega^2) \sin \alpha \, d\alpha.$$

From equations (6) and (8), the Gaussian width ω is found to be 0.42 rad. First we calculate the absorption coefficients associated with the perfectly ordered LC. We assume that each dye molecule has one absorption dipole only, that this is aligned at an angle β with respect to the long molecular axis, and that, in the molecular frame of reference, perpendicular to this axis there is no absorption. The total absorption coefficient, Δ , of the perfectly ordered LC is then given [13] by

$$\Delta = D_{\parallel} + 2D_{\perp} \quad (9)$$

where $D_{\parallel}$ and $D_{\perp}$ are the measured absorption coefficients parallel and perpendicular to the director. When the principal absorption axis of the dye molecules is at an angle β to their long axis, Saupe and Maier [13] also showed that

$$S = \frac{gN - 1}{(gN + 2)(1 - \frac{3}{2} \sin^2 \beta)} \quad (10)$$

where $N = D_{\parallel}/D_{\perp}$ and $g = n_e/n_o$. For the LC material whose specification is given in table 4, β is found to be zero. Therefore the principal absorption axis is parallel to the long molecular axis and molecular rotations about this axis do not affect the absorption coefficients. Then, on the basis of the previously stated assumption that the guest dye is isomorphic with host nematic, the parallel absorption coefficient, $\Delta_{\parallel}$, associated with the perfectly ordered LC is given by the right-hand side of (9) and the perpendicular absorption coefficient, $\Delta_{\perp}$, is zero.

Second, the refractive indices of the ordered structure are calculated using the equation relating refractive

Table 5. Perfectly ordered LC optical constants.

Parallel absorption coefficient, $\Delta_{\parallel}$	0.4712 μm^{-1}
Perpendicular absorption coefficient, $\Delta_{\perp}$	0
Extraordinary refractive index, ν_e	1.666
Ordinary refractive index, ν_o	1.485

index and orientation in a uniaxial medium [14]:

$$\nu_{\alpha}^2 = \nu_e^2 \cos^2 \alpha + \nu_o^2 \sin^2 \alpha. \quad (11)$$

If we average over all possible orientations by integrating the expression for ν_{α} , weighted by the probability density function in orientation $p_g(\alpha)$, the following coupled equations are obtained for the ordered refractive indices ν_e and ν_o :

$$\begin{aligned} n_e &= \int_{\alpha=0}^{\pi} \int_{\gamma=0}^{2\pi} p_g(\alpha) \nu_{\alpha} \sin \alpha \, d\alpha \, d\gamma \\ &= 4\pi \nu_o \int_0^{\pi/2} p_g(\alpha) (1 - K^2 \cos^2 \alpha)^{1/2} \sin \alpha \, d\alpha \end{aligned} \quad (12)$$

$$\begin{aligned} n_o &= \int_{\alpha=0}^{\pi} \int_{\gamma=0}^{2\pi} p_g(\alpha) [\nu_e \sin^2 \alpha \sin^2 \gamma + \nu_o^2 (\cos^2 \alpha \sin^2 \gamma \\ &\quad + \cos^2 \gamma)]^{1/2} \sin \alpha \, d\alpha \, d\gamma \\ &= 4\pi \nu_o \int_0^{\pi/2} p_g(\alpha) \Psi(K \sin \alpha) \sin \alpha \, d\alpha \end{aligned} \quad (13)$$

where

$$\begin{aligned} \Psi(x) &= 1 - \left(\frac{1}{2}\right)^2 \frac{x^2}{1} - \left(\frac{1.3}{2.4}\right)^2 \frac{x^4}{3} - \dots \\ &\quad - \left(\frac{(2N-1)!!}{2^N N!}\right)^2 \frac{x^{2N}}{(2N-1)} - \dots \end{aligned}$$

γ is the azimuthal angle and $K^2 = 1 - \nu_e^2/\nu_o^2$. The function $\Psi(x)$ arises in the context of complete elliptic integrals [15]. We may find K^2 and from this values of ν_e and ν_o by dividing equation (13) by equation (12) and using the bisection method. Table 5 lists the ordered LCs optical constants.

An alternative method, which avoids the introduction of $p_g(\alpha)$, is described by de Jeu [16]. In this method assumptions must be made about the relationship between the internal microscopic and external macroscopic electromagnetic field. The values predicted for ν_e and ν_o are 1.666 and 1.485 respectively, which agree well with those contained in table 5. However, the assumptions necessary to justify the model de Jeu describes are stronger than those necessary to justify the model described above.

5.2. Computational technique

The mean director orientation was computed, using the technique described in § 2, at each of 1000 points through the LC layer. This was done for a range of

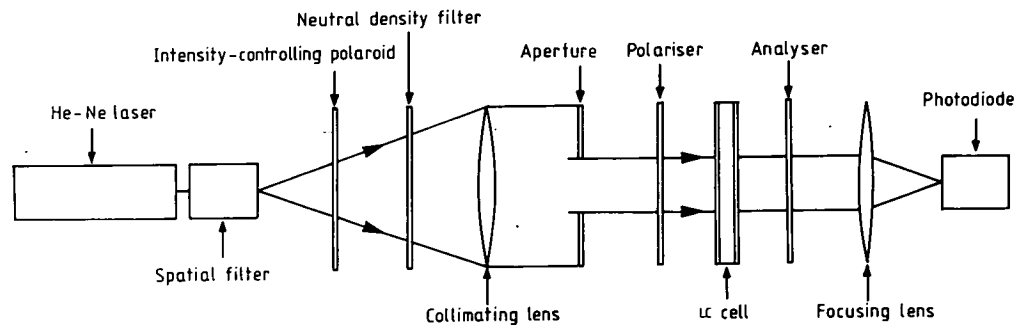


Figure 8. LC cell optical test bench.

voltages from threshold up to 7 V RMS and the results were stored in the form of look-up tables. These results were then used to compute the LC layer capacitance at different voltages as described in § 4. The capacitance values were substituted into the LC cell equivalent circuit shown in figure 6 to calculate the voltage across the cell corresponding to each voltage across the LC. Cell voltage is a much more useful quantity than LC voltage in this case because the optical properties predicted may be compared directly with experimental transmission measurements.

First, the transmission was computed, at each voltage, using the measured values of the complex refractive indices, assuming the director to be fixed in its mean orientation, as described in § 3. Secondly, the transmission was computed, taking account of the director fluctuations, in the following way

Within each of the 1000 slices of the LC layer, the optical axis was assumed to have probability density function in orientation $p_1(\alpha_i)$ about the mean calculated above. A random number generator [17] with probability density function $p_1(\alpha_i)$ was used to select a set of

orientational deviations from the mean, one for each slice. The tilt and twist angles were then calculated for each slice through the LC layer and, using the computed refractive indices, the cell's transmission computed. Another set of orientational deviations from the mean was selected randomly and the cell's transmission computed. The transmission of the cell for further random configurations was computed until the successive mean transmissions varied by less than 2%. Typically this condition was satisfied by taking the mean transmission from one hundred configurations.

The width of the local probability density function was varied to obtain a best fit with the transmission against cell-voltage curve measured experimentally.

6. Experimental measurements

A schematic diagram of the optical bench used for all experimental measurements is shown in figure 8. Light from a 5 mW He-Ne laser was passed through a spatial filter and collimated by a lens. The beam diameter was

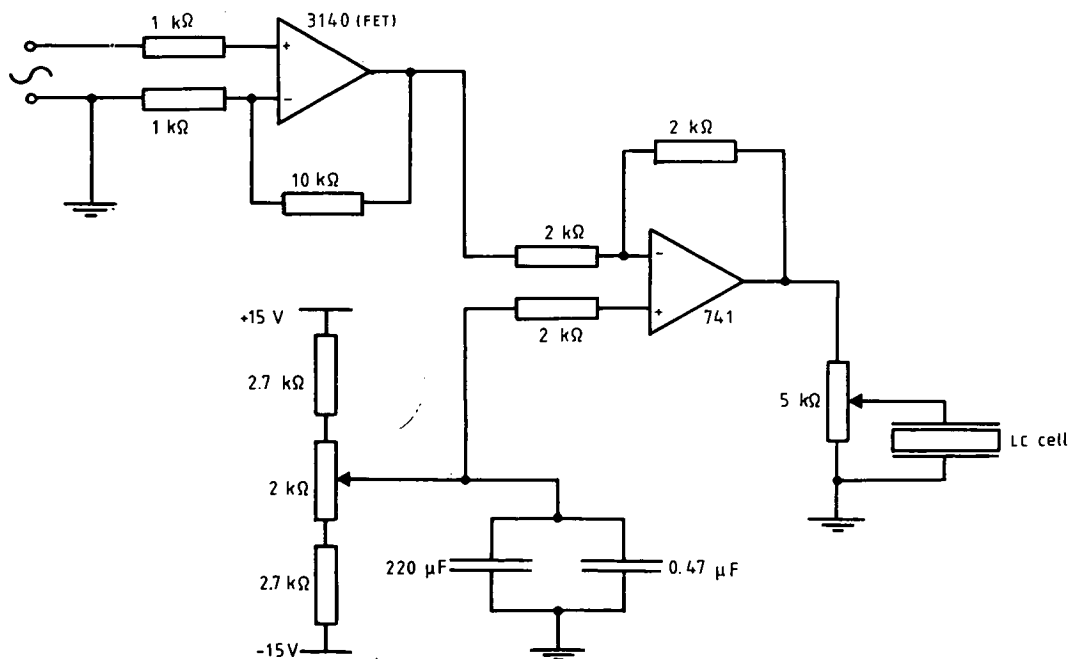


Figure 9. LC cell voltage control circuit.

reduced to 3 mm by an aperture and the light passed through a high-quality sheet polariser into the LC cell. Light transmitted through the cell was analysed by a second polariser and focused onto a photodiode by the second lens.

Voltage control for the LC cell was provided by the custom built amplifier and stepper-motor-controlled voltage divider (5 k Ω variable resistor) shown in figure 9.

The high input-impedance FET operational amplifier 3140 amplifies the input sinusoidal signal and the second stage acts as an inverting subtractor to remove any DC component from the amplified signal. A subtractor is included as any DC component would cause electrolytic decomposition of the LC. The LC cell voltage is controlled by a BBC-B microcomputer using a stepping motor to set the value of the resistance in parallel with the LC cell to any of 480 values between 0 and 5 k Ω . Output from the photodiode was fed through a signal conditioner to the BBC-B.

Sets of measurements of the transmission of the LC were made by increasing the LC voltage from zero to 20 V peak-to-peak in steps of about 42 mV and recording the light intensity after a pause of 0.5 s. The polariser was aligned with the LC front-face director by removing the analyser and finding the polariser orientation producing minimum transmission. To set the position of the analyser the LC cell was removed and the analyser oriented to give either maximum or minimum transmission. Experimentally measured transmissions are critically dependent upon the polaroid alignments relative to the LC cell.

7. Comparison of theory and experiment

Results are presented here for the experimentally measured transmission of a guest-host LC 13 μm thick. These results are compared with the theoretical predictions of the model described above, with and without the molecular disorder correction. The transmissions

are plotted in figure 10(a) and (b) for parallel and perpendicular polaroids.

In the corrected model the disorder factor σ was set to 1.2. The maximum iterative uncertainty is denoted by the vertical error bars. The relative scale factor for each pair of theoretical transmission curves (with and without the disorder correction) was chosen by eye to give the best overall fit to the experimental data over the range of voltages measured.

The overall correlation between theory and experiment is significantly improved when the molecular disorder correction is included. At larger voltages there is a small systematic error in the prediction of the corrected model. This is thought to arise principally because of the assumption that the orientational fluctuations are unaffected by the electric field. In practice, increasing the applied field suppresses these fluctuations so we might expect the uncorrected model to become more realistic. This would mean that in figure 10 the corrected theoretical curves would be closer than they are to the uncorrected curves at large fields. Then the corrected curves would match the experimental data better.

Acknowledgments

I thank Dr D G Vass and Dr R C Dougal for their support and encouragement throughout this work and other members of the Applied Optics Group for helpful discussions. Thanks are also due to Mr A Garrie for technical assistance in building the LC cells. Finally, the award of an SERC CASE studentship with STC Technology Ltd under the supervision of Mr W A Crossland is gratefully acknowledged.

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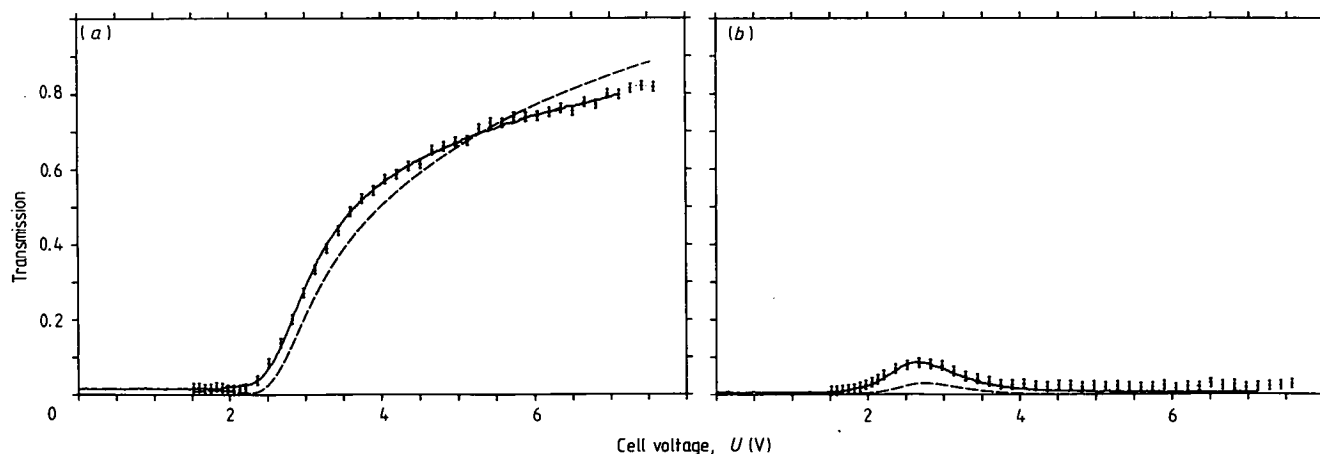


Figure 10. LC cell transmission through parallel polaroids (a) and perpendicular polaroids (b). In both cases the incident light was polarised parallel to the front-face director. The full curve is the experimental data, the broken curve the uncorrected model and the points with error bars the model including the molecular disorder correction.

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ERRATUM

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

Equation (11) mistakenly gives the formula for the ray velocity in a birefringent medium and should be replaced by the formula for the wave-front-normal velocity [18]

$$\frac{1}{\nu_\alpha^2} = \frac{\cos^2 \alpha}{\nu_e^2} + \frac{\sin^2 \alpha}{\nu_o^2} \tag{11}$$

Equations (12) and (13) then become

$$\begin{aligned} n_e &= \frac{\nu_e \nu_o}{4\pi Z_\omega} \int_{\alpha=0}^{\pi} \int_{\gamma=0}^{2\pi} \frac{\exp(-\alpha^2/\omega^2) \sin \alpha \, d\alpha \, d\gamma}{(\nu_e^2 \sin^2 \alpha + \nu_o^2 \cos^2 \alpha)^{1/2}} \\ &= \frac{\nu_o}{Z_\omega} \int_0^{\pi/2} \frac{\exp(-\alpha^2/\omega^2) \sin \alpha \, d\alpha}{(1 - K^2 \cos^2 \alpha)^{1/2}} \end{aligned} \tag{12}$$

$$\begin{aligned} n_o &= \frac{\nu_e \nu_o}{4\pi Z_\omega} \int_{\alpha=0}^{\pi} \int_{\gamma=0}^{2\pi} \exp(-\alpha^2/\omega^2) \\ &\quad \times \frac{\sin \alpha \, d\alpha \, d\gamma}{[\nu_e^2(\cos^2 \alpha \sin^2 \gamma + \cos^2 \gamma) + \nu_o^2 \sin^2 \alpha \sin^2 \gamma]^{1/2}} \\ &= \frac{\nu_o}{Z_\omega} \int_0^{\pi/2} \Psi(K \sin \alpha) \exp(-\alpha^2/\omega^2) \sin \alpha \, d\alpha \end{aligned} \tag{13}$$

where

$$\begin{aligned} \Psi(x) &= 1 + \left(\frac{1}{2}\right)^2 x^2 + \left(\frac{1.3}{2.4}\right)^2 x^4 + \dots \\ &\quad + \left(\frac{(2N-1)!!}{2^N N!}\right)^2 x^{2N} + \dots, \end{aligned}$$

γ is the azimuthal angle and $K^2 = 1 - \nu_o^2/\nu_e^2$. The solution of these equations for ν_e and ν_o is 1.666 and 1.485 respectively. These values are very similar to those predicted by de Jeu.

If the disorder factor σ is now set to 2.0 the following results are obtained.

Figure 10 should be replaced as below.

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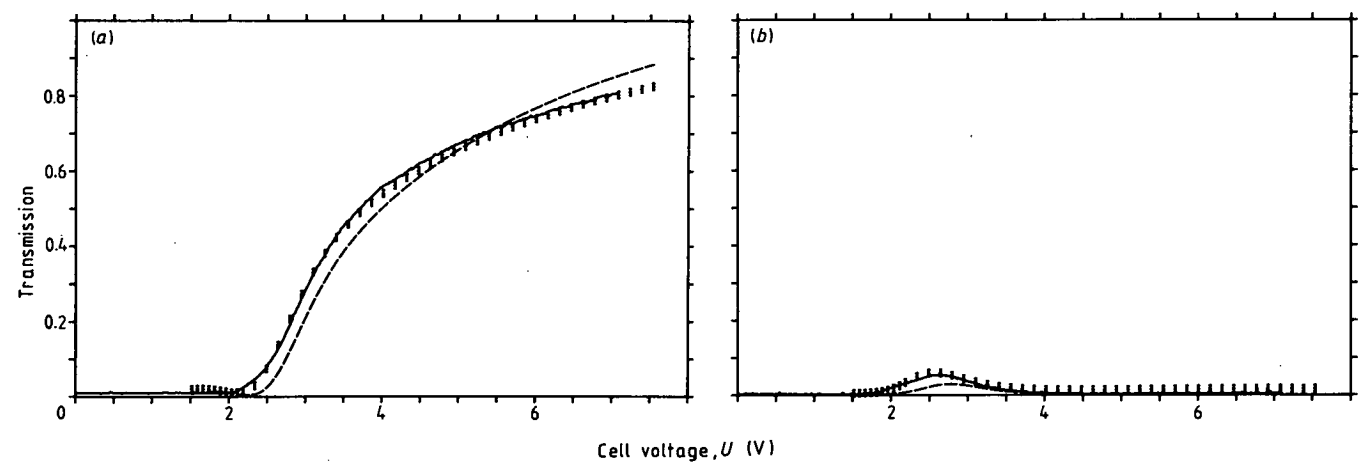


Figure 10. LC cell transmission through parallel polaroids (a) and perpendicular polaroids (b). In both cases the incident light was polarised parallel to the front-face director. The full curve is the experimental data, the broken curve the uncorrected model and the points with error bars the model including the molecular disorder correction.

A Method for Computing the Optical Properties of a Smectic C* Liquid Crystal Cell

Alastair R. MacGregor

Abstract

In the past, theoretical and experimental studies of ferroelectric chiral smectic C liquid crystals (SmC* LCs) concentrated on very thin (approximately $2\mu\text{m}$) devices which are difficult to build accurately. In this paper a formalism is presented for computing the director orientation in a cell containing SmC* LC. This formalism is applied to thicker, more easily constructed, LC cells and allows for interactions within and between the smectic layers which have not been considered in previous studies. Results of the director orientation calculations are presented and used in a formalism developed elsewhere [†] to compute the transmittance of a $7\mu\text{m}$ thick cell for different azimuthal orientations of the cell between crossed polarisers. It is shown that the theoretical and measured orientations which give minimum transmittance are in good agreement. Finally it is shown that the computed average-director-tilt angle is consistent with conoscopic measurements performed with a polarising microscope.

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1 Introduction

A great deal of interest has been shown recently in ferroelectric liquid crystals (LCs). These smectic LCs have shown considerable promise as fast electro-optic light modulators exhibiting bistability. High resolution flat panel displays[1] and spatial light modulators[2] have been built avoiding the need for an active matrix (where each pixel has its own circuitry). A large proportion of previous work on ferroelectric LCs, both theoretical and experimental, has been with LC cells of thickness $2\text{ }\mu\text{m}$ or less. It is much easier to build thicker cells reliably and it might be possible to use the same production lines as for nematic LC displays. In this paper a formalism is developed to describe thicker ($7\text{ }\mu\text{m}$) cells and this is used to examine some of their advantages and disadvantages over thin cells.

Smectic LCs are characterised by orientational order and varying degrees of positional order of their molecules. In a chiral smectic C (SmC^*) LC the molecules form a layered structure and tilt away from the layer normal by an angle θ (cf figure 1). The director, a unit vector $\mathbf{n}$, is defined as being the local mean molecular orientation and the projection of this onto the layer plane defines the orientation of the unit length c-director. In order to maintain the minimum-energy configuration, in which the smectic layers have constant spacing, the n-director may only move on the surface of a cone. As a result of the chirality of the SmC^* molecules the n-director precesses about the cone from layer to layer. In addition the chirality reduces molecular symmetry within each layer in such a way as to align the molecules' transverse dipoles[3, chapter 7]. The resultant spontaneous polarisation $\mathbf{P}_s$ lies perpendicular to the c-director and in the layer plane as shown in figure 1. Thus, within each layer, SmC^* LCs are ferroelectric though the orientation of $\mathbf{P}_s$ precesses from layer to layer.

SmC^* liquid crystals, though biaxial, may to a good approximation[4] be considered uniaxial. The n-director is parallel to the local optic axis of the medium. In order to produce a uniform electro-optic effect the helical structure must first be unwound. Clark and Lagerwall[5] first did this using the so-called surface stabilised ferroelectric LC (SSFLC) geometry in which the LC is sandwiched between two glass plates spaced approximately $1\text{ }\mu\text{m}$ apart as shown in figure 2. In this geometry the LC has two stable director configurations one with $\mathbf{P}_s$ pointing up and the other with $\mathbf{P}_s$ pointing down. Bistable switching from one to the other is achieved by applying a d.c. voltage pulse across the indium tin oxide (ITO) electrodes. Optical contrast is produced by placing the LC cell between crossed polaroids and aligning the n-director of one state with the axis of the front polariser.

SSFLC devices have switching times several orders of magnitude faster than the best nematic LC devices; this is because in the ferroelectric devices the electric field couples directly to the spontaneous polarisation whereas in the nematic devices the field interacts with the dielectric anisotropy of the medium. There are however two major problems with these SmC^* devices. Firstly it is very difficult to make them flat when they are so thin and secondly the LC must have a large birefringence if it is to act as a half-wave plate and so satisfy the condition for optimum contrast[6, chapter 14.4]. If thicker cells are used then both of these restrictions may be relaxed, although thicker cells suffer from less effective surface stabilisation. In this paper the director configurations which occur in thicker cells are calculated and used to investigate how the behaviour of a thick cell differs from that described above.

Elastic continuum theories have been used widely in the study of both nematic and smectic liquid crystals. Minimisation of the free energy functions generated by these theories enables calculation of the director configurations. A survey of the functions which have been used to describe SmC* LCs is provided by Akahane and Nakagawa[7]. In all of them however the smectic layers were assumed to be planar, either perpendicular to the glass surfaces or tilted at a constant angle to them. *A priori* there is no reason why these layers should have a fixed orientation or indeed be planar at all. De Gennes[3, chapter 7] has derived a general expression for the free energy density of SmC* LCs which takes account of layer distortions as well as director distortions within layers. His expression, reformulated by Dahl and Lagerwall[8], is used in this paper along with an improved form of the surface interaction energy function to compute the director configuration in a 7 μm thick cell. The method used to find the minimum-energy configuration takes into account the contribution of the polarisation field to the local electric field and the way in which this local field interacts with both the spontaneous and induced polarisations of the molecules. The transmittance of a 7 μm thick cell for different azimuthal orientations of the cell between crossed polarisers is then computed using the 4×4 matrix method of Berreman[9]. The theoretical and measured azimuthal orientations which give minimum transmittance are shown to be in good agreement. Finally it is shown that the computed-average-tilt angle is consistent with conoscopic measurements performed with a polarising microscope.

2 Theory

In this section the equations used to describe the free energy of bulk LC distortions, surface interactions and field interactions are presented. First of all, the coordinate system used in the theoretical formulation is shown in figure 3. In the xyz coordinate system (figure 3a; cf figure 2) the x -axis is normal to the bounding plates and the z -axis corresponds to the rubbing direction of the nylon surface treatment (see section 5.1 for details). It is observed experimentally that the two stable states of the LC are symmetrically positioned about the xz -plane. Therefore it was assumed that the unit vector $\mathbf{k}$, describing the layer normal at any point, could be uniquely described by the angle ψ (figure 3b). This angle relates the xyz coordinate system to the $x'yz'$ system in which the c -director orientation is specified by the angle ϕ (figure 3c). It was also assumed that, since the LC cell appeared uniform in optical texture, $\mathbf{c}$ and $\mathbf{k}$ varied only in the x -direction. In the xyz coordinate system the $\mathbf{c}$ and $\mathbf{k}$ vectors are given by

$$\mathbf{c} = (-\cos \psi \sin \phi, \cos \phi, \sin \psi \sin \phi), \quad (1)$$

$$\mathbf{k} = (\sin \psi, 0, \cos \psi). \quad (2)$$

These vectors are orthonormal and together describe all possible $\mathbf{c}$ and $\mathbf{k}$ orientations. The two angles ϕ and ψ also uniquely define the director orientations. Within this coordinate system the unit vector $\mathbf{p}$ defining the direction of the spontaneous polarisation $\mathbf{P}_s$ is given by

$$\mathbf{p} = \mathbf{k} \times \mathbf{c}. \quad (3)$$

Using the definitions (1) and (2) allows us to compute $\mathbf{n}$ with the following expression

$$\mathbf{n} = \mathbf{k} \cos \theta + \mathbf{c} \sin \theta. \quad (4)$$

Equation (4) then allows us to compute the tilt angle β and azimuthal angle α thus:

$$\sin \beta = n_x = \sin \psi \cos \theta - \cos \psi \sin \phi \sin \theta, \quad (5)$$

$$\sin \alpha = \frac{n_y}{\cos \beta} = \frac{\cos \phi \sin \theta}{\cos \beta}. \quad (6)$$

These coordinate systems enable us to derive the appropriate form for the free energy density. de Gennes[3, chapter 7] has derived a general expression for the elastic free energy density of a SmC* LC. This has been reformulated by Dahl and Lagerwall[8] in terms of the vectors $\mathbf{c}$ and $\mathbf{k}$. Substituting equations (1) and (2) into their equations 7 to 11 we obtain the following expression for the elastic free energy density:

$$f_{elas} = f_c + f_s + f_{cs} + f_* \quad (7)$$

where f_c is the contribution from $\mathbf{c}$ -director distortions, f_s is from the layer distortions, f_{cs} is from the coupling between $\mathbf{c}$ -director and layer distortions and f_* is the chiral elastic contribution. In terms of the angles ϕ and ψ defined above:

$$f_c = \frac{1}{2}B_1[\phi_x \cos \psi \sin \phi]^2 + \frac{1}{2}B_2[\psi_x \sin \psi \sin \phi - \phi_x \cos \psi \cos \phi]^2 + \frac{1}{2}B_3[\phi_x \sin \psi]^2 - B_{13}\phi_x^2 \cos \psi \sin \psi \sin \phi, \quad (8)$$

$$f_s = \frac{1}{2}A_{11}[\psi_x \cos \psi \cos \phi \sin \phi]^2 + \frac{1}{2}A_{12}[\psi_x \cos \psi \sin^2 \phi]^2 + \frac{1}{2}A_{21}[\psi_x \cos \psi \cos^2 \phi]^2, \quad (9)$$

$$f_{cs} = C_1\psi_x\phi_x\cos^2\psi\cos\phi\sin^2\phi - C_2\psi_x\cos\psi\cos^2\phi[\psi_x\sin\psi\sin\phi - \phi_x\cos\psi\cos\phi], \quad (10)$$

$$f_* = D\phi_x\sin\psi - D_1\phi_x\cos\psi\sin\phi - D_2\psi_x\cos\psi\cos\phi\sin\phi, \quad (11)$$

where each subscript x denotes the operation $\partial/\partial x$. In equation (8) the B_1, B_2 and B_3 terms correspond to bend, splay and twist distortions of the $\mathbf{c}$ -director while the B_{13} term corresponds to the coupling between bend and twist distortions of the $\mathbf{c}$ -director. The A and C constants in equations (9) and (10) correspond to layer distortions and coupling between $\mathbf{c}$ -director and layer distortions respectively. In equation (11) the D term produces the $\mathbf{c}$ -director twist shown in figure 1, the D_1 term tries to produce a constant bend of the $\mathbf{c}$ -director and the D_2 term couples $\mathbf{c}$ -director twist to layer bending. Values of these elastic constants can be estimated in terms of the Frank elastic constants of nematic theory and the helical pitch of the $\mathbf{c}$ -director in a bulk LC sample as shown in section 3.2.

Next we consider the contribution to the free energy density arising from the interaction of the LC with a static electric field. The contribution associated with the induced dipoles, the dielectric free energy density, is given by

$$f_d = -\frac{1}{2}\epsilon_{xx} \left(\frac{\partial \Phi}{\partial x} \right)^2 \quad (12)$$

where Φ is the electric scalar potential which is related to the x -component of the electric field by $E_x = -\partial\Phi/\partial x$. ϵ_{xx} is the component of the dielectric ellipsoid parallel to the x -axis which is given by

$$\epsilon_{xx} = \epsilon_o\epsilon_{\perp}(1 + e \sin^2 \beta) \quad (13)$$

where $e = (\epsilon_{\parallel} - \epsilon_{\perp})/\epsilon_{\perp}$ and $\epsilon_{\parallel}$ and $\epsilon_{\perp}$ are the principal dielectric constants along the $\mathbf{n}$ -director and perpendicular to it. The contribution to the free energy density

associated with the interaction of the electric field $\mathbf{E}$ with the spontaneous polarisation $\mathbf{P}_s$ is given by

$$f_p = -P_s \cos \psi \cos \phi \left(\frac{\partial \Phi}{\partial x} \right). \quad (14)$$

Finally we consider the contribution to the total free energy arising from the interaction of the LC with its bounding surfaces. Two terms are considered: the first is of the general type used by Nakagawa *et al.* [10] and the second a nematic type of surface interaction. Together they encourage a uniform layer tilt across the cell with the surface $\mathbf{n}$ -director parallel to the surface in one of two positions symmetrically positioned either side of the rubbing direction. A tilted layer formation is thought to be produced by the layer shrinkage which occurs on cooling the LC from the smectic A to SmC* phase [11].

It was assumed that the surface free energy per unit area was

$$f_{surf} = -\sigma_1 f_1(\phi) - \sigma_2 f_2(\beta) \quad (15)$$

where

$$f_1(\phi) = \begin{cases} \exp\left(-\gamma \sin^2\left(\frac{\phi_1}{2}\right)\right) & \text{if } \phi \notin [2m\pi + \phi_o, (2m+1)\pi - \phi_o] \\ \left(\frac{\pi - 2\phi_o}{\pi + 2\phi_o}\right) \sin^2 \phi_2 & \text{otherwise,} \end{cases}$$

where

$$\begin{aligned} \phi_1 &= \left(\frac{2\pi}{\pi + 2\phi_o} \right) [\phi - ((2m+1)\pi - \phi_o)] \\ \phi_2 &= \left(\frac{\pi}{\pi - 2\phi_o} \right) [\phi - (2m\pi + \phi_o)] \end{aligned}$$

and

$$f_2(\beta) = \exp(-\gamma \sin^2 \beta). \quad (16)$$

In the above m is any integer, γ is a constant which controls the steepness of the potential wells in the surface-potential functions and ϕ_o defines the positions of the minima in $f_1(\phi)$. Figure 4 shows the form these functions take for some typical values of γ and ϕ_o . The value of ϕ_o was determined approximately from experimental measurements (cf section 5.1) of the zero-field apparent azimuthal angle using equation (6) and assuming no surface pretilt i.e. $\beta = 0$. Although the mathematical form of f_{surf} is not derived physically it does reproduce the observed physical behaviour and was therefore used as a first approximation. The total free energy is thus given by

$$F(\phi, \psi; \Phi) = \int_v f_{vol} dv + \int_s f_{surf} ds = \int_v (f_{elas} + f_d + f_p) dv + \int_s f_{surf} ds. \quad (17)$$

3 Calculating the Free Energy Configuration

3.1 Minimising the Free Energy Function

In this section we solve the free energy equation (17) to find the minimum energy director configuration. Although we are only concerned with static director configurations

it is convenient to introduce pseudo-viscosities for the rotation of both $\mathbf{c}$ and $\mathbf{k}$. A time-dependent formulation of the solution was chosen because the associated iteration method is stable for any combination of elastic constants. However it might be possible to interpret the pseudo viscosities as real viscosities and calculate dynamic director configurations [10]. The bulk torque balance equations may then be written as

$$\eta_v \frac{\partial \phi}{\partial t} = - \left[\frac{\partial f_{\text{vol}}}{\partial \phi} - \frac{\partial}{\partial x} \left(\frac{\partial f_{\text{vol}}}{\partial \phi_x} \right) \right], (0 < x < d), \quad (18)$$

$$\eta_v \frac{\partial \psi}{\partial t} = - \left[\frac{\partial f_{\text{vol}}}{\partial \psi} - \frac{\partial}{\partial x} \left(\frac{\partial f_{\text{vol}}}{\partial \psi_x} \right) \right], (0 < x < d). \quad (19)$$

The surface torque balance equations are

$$\eta_s \frac{\partial \phi}{\partial t} = - \left[\frac{\partial f_{\text{surf}}}{\partial \phi} - (\mathbf{x} \cdot \mathbf{s}) \frac{\partial f_{\text{vol}}}{\partial \phi_x} \right], (x = 0, d), \quad (20)$$

$$\eta_s \frac{\partial \psi}{\partial t} = - \left[\frac{\partial f_{\text{surf}}}{\partial \psi} - (\mathbf{x} \cdot \mathbf{s}) \frac{\partial f_{\text{vol}}}{\partial \psi_x} \right], (x = 0, d). \quad (21)$$

Equations (18)-(21) are in the form of multi-variable TDGL[12] (time dependent Ginzburg Landau) equations. In them η_v is the bulk rotational viscosity of both $\mathbf{c}$ and $\mathbf{k}$ while η_s is the surface rotational viscosity. The $\mathbf{c}$ and $\mathbf{k}$ viscosities were assumed equal for convenience but in general would be different. In equations (20) and (21) $\mathbf{s}$ is the unit surface normal pointing into the LC at each surface and $\mathbf{x}$ is the unit vector in the x -direction. In the torque-balance equations the terms involving the viscosities vanish for the steady-state solutions and the values of the viscosities simply control the rate of convergence to that solution. Substituting equation (17) into (18) to (21) we obtain the following simultaneous coupled partial differential equations:

$$\eta_v \frac{\partial \phi}{\partial t} = - [\Gamma_1 \phi_{xx} + \Gamma_2 \psi_{xx} + \Gamma_3 \phi_x^2 + \Gamma_4 \psi_x^2 + \Gamma_5 \psi_x \phi_x + \Gamma_6 \psi_x + \Gamma_7], \quad (22)$$

$$\eta_v \frac{\partial \psi}{\partial t} = - [\Lambda_1 \psi_{xx} + \Lambda_2 \phi_{xx} + \Lambda_3 \phi_x^2 + \Lambda_4 \psi_x^2 + \Lambda_5 \psi_x \phi_x + \Lambda_6 \phi_x + \Lambda_7], \quad (23)$$

$$\eta_s \frac{\partial \phi}{\partial t} = (\mathbf{x} \cdot \mathbf{s}) [\Gamma_8 \phi_x + \Gamma_9 \psi_x + \Gamma_{10}] - \Gamma_{11}, \quad (24)$$

$$\eta_s \frac{\partial \psi}{\partial t} = (\mathbf{x} \cdot \mathbf{s}) [\Lambda_8 \psi_x + \Lambda_9 \phi_x + \Lambda_{10}] - \Lambda_{11}. \quad (25)$$

The form of the Γ_i and Λ_i is given in the appendix.

Before we can solve these equations we must first calculate the local electric field strength within the LC taking into account the polarisation field produced by the spontaneous polarisation $\mathbf{P}_s$. The polarisation field is particularly important when small external fields are applied, as shown by Nakagawa *et al.*[13], as it has the effect of reducing the local electric field strength where there is a large rate of change of the orientation of $\mathbf{P}_s$. Introducing a pseudo-viscosity η_Φ we can minimise the volume free energy with respect to Φ as for ϕ and ψ . For a particular director configuration, Φ is obtained by finding the steady-state solution of

$$\eta_\Phi \frac{\partial \Phi}{\partial t} = - \left[\frac{\partial f_{\text{vol}}}{\partial \Phi} - \frac{\partial}{\partial x} \left(\frac{\partial f_{\text{vol}}}{\partial \Phi_x} \right) \right], (0 < x < d) \quad (26)$$

subject to the boundary conditions that $\Phi(0) = 0$ and $\Phi(d) = V$ (where V is the voltage applied across the cell). Substituting equation (17) into (26) we obtain

$$\eta_\Phi \frac{\partial \Phi}{\partial t} = - \left[\frac{\partial}{\partial x} \left(\epsilon_o \epsilon_\perp (1 + e \sin^2 \beta) \frac{\partial \Phi}{\partial x} \right) - P_s (\psi_x \sin \psi \cos \phi + \phi_x \cos \psi \sin \phi) \right]. \quad (27)$$

The solution to this equation shows how the scalar potential varies as a function of x .

In order to calculate the director configuration across the cell we first replace all the derivatives in equations (22) to (25) and (27) by finite differences. Then we divide the x -axis into N divisions. For a cell of thickness $7\mu m$ N was set to 72. If we denote a division of the x -axis by Δx then the time division Δt must satisfy certain conditions to ensure convergence of the iterative method[14, chapter 10.2]. Equations (22) to (25) will converge provided that:

$$\left(\frac{\Delta t}{\eta_v(\Delta x)^2}\right) \max(A_{11}, A_{12}, A_{21}, B_1, B_2, B_3, B_{13}, C_1, C_2) < 0.5 \quad (28)$$

where the function $\max$ selects the largest one of its arguments. The bulk rotational viscosity was taken to be $10^{-2} Pa.s$ and the time step Δt chosen to make the left-hand-side of equation (28) equal to 0.1. η_s , the surface rotational viscosity was taken to be $\eta_v \Delta x$. Convergence of equation (27) requires that

$$\frac{\Delta t \epsilon_o \epsilon_{\perp} e}{\eta_s (\Delta x)^2} < 0.5 \quad (29)$$

so η_s was chosen to make the left hand side of inequality (29) equal to 0.1. Once $\Delta x, \Delta t$ and the viscosities had been selected the starting configuration was chosen to be $\phi(x) = \psi(x) = 0$ for which $\Phi(x) = xV/d$. The fourth order Runge-Kutta (R-K)[14, chapter 9] method was then used to solve equations (22)–(25). After each time step the scalar potential was evaluated by solving equation (27) also using the fourth order R-K method.

3.2 Estimating Values for the Elastic Constants

This subsection explains the way in which values for the elastic constants in the free energy equation were estimated. The first method used was to compare the form of the elastic free energy density used here with a nematic-like expression and to estimate the values of the constants from those measured for nematic LCs. This comparison requires that the layer normal is constant. It was assumed to be so to estimate the values of the elastic constants but was subsequently allowed to vary. Handschy *et al.*[15] proposed a simple extension of the nematic elastic free energy density to describe SmC* LCs:

$$f = \frac{1}{2}K_1(\nabla \cdot \mathbf{n})^2 + \frac{1}{2}K_2(\mathbf{n} \cdot \nabla \times \mathbf{n} + q_{||})^2 + \frac{1}{2}K_3(\mathbf{n} \times \nabla \times \mathbf{n} + \mathbf{q}_{\perp})^2, \quad (30)$$

where $q_{||}$ denotes the spontaneous twist and the vector $\mathbf{q}_{\perp}$ denotes the spontaneous bend of the $\mathbf{n}$ -director. If we assume that k is constant through the LC in equation (7) and we set $K_1 = K_2 = K_3 = K$ then it can be shown [7] that $B_1 = B_2 = B_3 = K \sin^2 \theta = B$ and $B_{13} = 0$. In a typical nematic LC K is of order $10^{-11} N$ so we expect B to be somewhat greater than $10^{-12} N$. When all the K_i constants are set equal equation (30) is minimised for $\phi = q_o z$ where q_o is given [7] by

$$q_o = \frac{-D}{K \sin^2 \theta}. \quad (31)$$

In this equation $q_o = 2\pi/p_o$ and p_o is the pitch of the helix shown in figure 1. The pitch of the helix can be measured directly (see section 5.3) and has a value of $5.8 \mu m$ for

the LC SCE3 at 15°C. Therefore we can estimate the value of D from equation (31). The significance of the sign is in determining the sense in which the helix is wound.

In the following analysis it was assumed that the layer bend elastic constants were all equal and had the same value as the B elastic constants i.e. $A_{11} = A_{12} = A_{21} = B$ and that as a first approximation the C elastic constants could be set to zero. The elastic constants D_1 and D_2 were set equal to the modulus of the value of D computed using equation (31). It was also assumed that the surface elastic constants were equal i.e. $\sigma_1 = \sigma_2 = \sigma$. Therefore the entire set of elastic constants was specified by choosing values of B , σ and γ . For these values the director configuration was calculated, and from this certain optical properties of the LC cell as described in the next section. A parameter survey was then performed to find the best fit to the experimentally measured optical properties.

4 Calculating LC Cell Optical Properties

This section describes the way in which the theory developed in sections 2 and 3 was used to simulate some of the optical properties of a SmC* LC cell. The first simulation is trivially performed once the director configuration has been calculated. It consists of calculating the average tilt angle $\bar{\beta}$ and comparing it with the value of $\bar{\beta}$ measured from the conoscopic figure of the cell as described in section 5.2. The second simulation allows comparison of the predicted values of the azimuthal angle α with those observed experimentally. In particular a simulation is performed where the cell is positioned between crossed polaroids and rotated about the x -axis until the minimum-transmission orientation is found. This orientation defines the apparent azimuthal angle α_{app} for the whole cell. The computed variation of α_{app} with voltage is compared with experimentally measured values and further tests the theory.

The conoscopic image (section 5.2) is determined by the effective birefringence of the LC layer and its azimuthal orientation relative to the polarisers. In a non-uniform sample the conoscopic figure will depend on the birefringence at every point through the sample. The total phase difference introduced along a particular path will be the integral of the phase differences along that path. When no voltage is applied to the LC cell the Mauguin limit for waveguiding is satisfied so, to a first approximation, no mixing of ordinary and extraordinary waves occurs. Therefore the total phase difference for a particular angle of incidence may be calculated by integrating along the ordinary and extraordinary wave-paths separately and taking the difference of the integrated values. For normally incident light the effective ordinary and extraordinary refractive indices are n_o and [16, chapter 6]

$$n_{eff} = \frac{n_e n_o}{\sqrt{n_e^2 \sin^2 \beta + n_o^2 \cos^2 \beta}} \quad (32)$$

where β is the tilt angle and n_e and n_o are the extraordinary and ordinary refractive indices of the medium. A numerical integration is then performed, using the computed values of β , to calculate the total phase difference Δ across the cell. It was assumed that the conoscopic figure which would be produced by the computed director structure would be the same as that due to a uniform LC layer whose tilt angle $\bar{\beta}$ was chosen to give the same value of Δ for normally incident light. This assumption is reasonable

provided that the director distortions are small, which they are when no electric field is applied. The computed value of $\bar{\beta}$ may then be compared with the tilt angle measured from the actual conoscopic figure.

In the second simulation the technique described by Montgomery [17,18] was applied to the cell shown schematically in figure 5 to calculate the transmission of the cell rotated by an angle η between crossed polaroids. Table 1 gives the dimensions of the LC cell used in the calculations. The value of η was altered to minimise the transmitted intensity. Montgomery's technique yields a solution to Maxwell's equations for the complete cell shown in figure 5. The method divides up the LC layer into slices so thin that the variation in optical properties across each layer becomes negligible (approximately one hundred slices per micron of cell thickness [19]). A cubic spline was fitted to the ϕ and ψ values calculated in section 3 to evaluate the director orientation for a total of 720 slices across the $7 \mu m$ cell. Table 2 lists the values of the optical constants used in the calculations.

The principle underlying the second simulation is illustrated by placing a birefringent slab between crossed polaroids. The transmitted intensity is given by

$$I = I_o \sin^2(2\eta) \sin^2 \left(\frac{\pi(n_{eff} - n_o)d}{\lambda} \right) \quad (33)$$

where I_o is the incident intensity, η is the angle which the optic axis makes with the front polariser axis, d is the sample thickness and λ is the wavelength of the light in vacuo. The orientation of the projection of the optic axis onto the plane of the slab is found by rotating the slab until the minimum transmission orientation is found. The projection of the optic axis is then aligned with the polariser axis. In general in a LC the optic axis varies in orientation throughout the sample and may not waveguide the light. However the value of η which gives minimum transmission, which we define to be the apparent azimuthal angle α_{app} , does yield an apparent value for the orientation of the optic axis, a parameter which may be readily measured.

In summary, simulations of the value of the average tilt angle $\bar{\beta}$ and the variation of apparent azimuthal angle α_{app} with applied voltage provide us with two experimentally verifiable predictions of the theory proposed in this paper. Before looking in detail at the results of the simulations the experimental techniques employed are presented.

5 Experimental Measurements

5.1 Measuring the Apparent Azimuthal Angle

The construction of the LC cell used is shown schematically in figure 5. Each of the ITO-coated glass plates was spin-coated with nylon and rubbed unidirectionally with lens tissue wrapped around a 20 mm diameter cylinder. Short sections of $7 \mu m$ diameter glass fiber rod were spread evenly over the lower plate to space the plates a uniform distance apart with the rubbing directions parallel. In all of the following experiments the B.D.H. liquid crystal SCE3 was used. Table 3 lists some of the physical properties of this material which exhibits the following phase transitions at the temperatures shown:

$$\longrightarrow < -20^\circ C \xleftrightarrow{SmC^*} 74^\circ C \xleftrightarrow{SmA} 105^\circ C \xleftrightarrow{N^*} 136^\circ C \xleftarrow{I}. \quad (34)$$

In equation (34) SmA stands for the smectic A phase, N^* stands for a chiral nematic phase and I for the isotropic phase. To ensure good alignment the manufacturers have adjusted the nematic pitch so as to be as near infinity as possible at the $SmA \longleftrightarrow N^*$ phase transition temperature. The empty cell was first heated to above the nematic-isotropic transition temperature and then filled by capillary action. After allowing the cell to cool to room temperature it was sealed with epoxy resin on all four sides. Uniform director alignment was produced by heating the complete cell into the nematic phase and cooling it very slowly into the SmA phase and finally into the SmC^* phase. From a number of such cells one was selected which had an even optical texture and uniform birefringence colour over its entire surface area.

Figure 6 shows schematically the optical bench used to measure the apparent azimuthal angle of the LC cell. A sodium discharge lamp was used as the light source as available refractive index data for SCE3 had been measured for the sodium-D spectral lines. The collimator consisted of a condenser lens, a 1mm diameter pinhole and a collimating lens. An iris diaphragm was used to reduce the beam diameter to 3mm and the light passed through high quality sheet polarisers placed either side of the LC cell. Light transmitted through the system with the polaroids crossed was focused onto a photodiode and the output monitored by a digital voltmeter. A bipolar square-wave voltage was applied across the cell to avoid the electrolytic degradation accompanying prolonged application of d.c. voltages. The amplitude of the signal could be set anywhere in the range 0 – 20V using a voltage divider while the frequency of the waveform was set to 0.1 Hz to allow measurement of d.c. field effects on the optical properties of the cell. A rotatable mount with a vernier scale calibrated to 0.1° was used to clamp the LC cell in position on the optical bench.

Measurement of the apparent azimuthal angle for a particular voltage amplitude was made by noting the minimum transmission orientation for each voltage polarity. As far as could be seen these two orientations were symmetrically positioned on either side of the rubbing direction. The positions of the minima were determined to within an absolute error of 0.5° and the apparent azimuthal angle calculated by halving the difference between the two angles. For voltages of 1V or less the measurements were made using d.c. voltages. To make sure that the whole cell was in a single state the voltage was initially set to about 5V and reduced to the required value.

The apparatus described above was also used to check the cell thickness. First the cell was driven into one state and the voltage reduced to zero. An optically uniform and defect-free texture indicated that the cell was in a single state. Then the minimum transmission orientation was located and a Babinet-Soleil compensator inserted into the light beam behind the LC cell. The compensator was set to give a retardation of about 100 nm and rotated until the minimum transmission orientation was found. To make sure that the extraordinary axes of the LC and compensator were crossed it was checked that the inclusion of the compensator produced a birefringence colour [20, chapter 9] equivalent to a smaller retardation than that of the LC alone. A retardation of $1.348\mu m$ was measured which, for a birefringence of 0.19, indicates a cell thickness of $7.1\mu m$ in good agreement with that expected. This was a rough check because it presupposed that the LC waveguides the light and also that the n-director was always parallel to the cell walls. However, on the basis of the theoretical director structures calculated these assumptions were reasonable.

5.2 Conoscopic Measurements

Conoscopic figures are usually observed using a polarising microscope [16, chapter 4]. A parallel beam of light is passed through a polariser, a condensing lens, the sample, the objective lens and an analyser which is crossed with respect to the polariser, emerging as a parallel beam. The conoscopic image is formed by the interference of the ordinary and extraordinary waves in the back focal plane of the objective lens. In a polarising microscope the Bertrand lens is inserted so that the ocular produces an image of the conoscopic figure. When observed using white light the figure is described in terms of isochromes and isogyres. Isochromes are lines of equal colour and isogyres are parts of the figure where extinction occurs. Both isochromes and isogyres yield information about the orientation of the optic axis/axes of the medium. In particular for a uniaxial sample the pattern of the isogyres and the way in which this pattern moves when the sample is rotated provides information about the angle at which the optic axis is tilted with respect to the plane of section. Although SmC* LCs are in fact slightly biaxial to a good approximation they may be considered to be uniaxial [4] and their consoscopic figures interpreted accordingly.

A high-powered objective lens was used to gather as wide a cone of light as possible from the sample and maximise the contrast of the isogyres. All observations were made using a Leitz Ortholux 2 Pol.-Ek. with a 50 $\times$ objective and 10 $\times$ eyepieces. The working distance of the objective lens was approximately 0.4mm which required a special LC cell to be made using a 0.1mm thick microscope cover glass as the upper surface of the cell. Figure 7 shows the “symmetric flash figure” [21, chapter 7] which was observed by rotating the sample on the microscope stage. The top and bottom images were obtained by rotating the sample 1.5 $^\circ$ away from the position in which the middle image was obtained. In these photographs the isogyres are the dark regions while the isochromes are not visible in the black and white photographs. A “symmetric flash figure” shows that the mean orientation of the optic axis is parallel to the glass plates to within a few degrees.

5.3 Helical Pitch Measurement

In section 3.2 it was shown that the strength of the chiral elastic constant D depends upon the pitch of the helical structure occurring in a bulk sample of SmC* LC. If the LC is contained within a thick cell (say 100 μm) then the surfaces produce homogeneous alignment of the n -director in their vicinity. However the surface interactions are insufficient to unwind the helix in the middle of the cell. These two structures are incompatible and lead to a regular distribution of linear defects as shown by Glogarova *et al.* [22]. These defects run parallel to the smectic layers and are clearly visible in both polarised and unpolarised light. Figure 8 shows these dechiralisation lines in a 100 μm cell containing the LC SCE3. The separation of these lines is precisely one helical pitch length and was measured using a graticule to be 5.8 μm at 15 $^\circ$ C. This value was subsequently used in the calculation of the value of the D constant.

6 Simulation Results and Comparison with Experimental Results

It was observed experimentally that the apparent azimuthal angle in a $7\ \mu\text{m}$ cell containing SCE3 was 1.5° when no voltage was applied to the cell. Subject to the assumptions made in section 2 the value of ϕ_o was determined using equation (6). Then, using the data in tables 1 and 2 the theoretical model described in sections 2 to 4 was applied to a $7\ \mu\text{m}$ cell to predict the ϕ and ψ configurations for different cell voltages. Figure 9 shows the predicted variations of ϕ and ψ through the cell. The effect of the chiral elastic energy is also demonstrated by showing the ϕ and ψ variation when there is no chiral energy. In these calculations the following values were used: $B = 6 \times 10^{-12}\ \text{N}$, $\sigma = 4.5 \times 10^{-5}\ \text{N}$, $\phi_o = 86.5^\circ$ and $\gamma = 5$.

Figure 10 shows the variation in apparent azimuthal angle with voltage, calculated from the predicted variation in ϕ and ψ , along with the experimentally measured values. The correspondence between theory and experiment is seen to be excellent. In addition it was noted that the calculated mean tilt angle, $\bar{\beta}$, was 0.1° which agrees well with the conoscopic data.

The static properties of a SSFLC device are summarised in equation (33). Optimum performance is obtained when the difference in orientation between the two states (2η) is 45° and the effective birefringence is such that the device behaves like a half-wave plate. If a low birefringence LC is used in a thick cell then the device performance is less sensitive to absolute variations in thickness than a high birefringence LC in a thin cell. However the zero-field value of η is only 1.5° in a $7\ \mu\text{m}$ cell compared to more than 10° in a $2\ \mu\text{m}$ cell. This effect could be related to the recently discovered "chevron" layer structure [11]. The contrast ratio between the two states is therefore much lower in thick cells than in thin cells, even when η is increased by a.c. stabilisation [23]. It is suggested therefore, that in applications requiring high contrast over relatively small areas, such as spatial light modulators, thin cells should continue to be used, but that in large-area displays where contrast is less important, thicker cells might give better optical uniformity and appearance.

In summary, a model has been proposed to describe the optical properties of a SSFLC cell of a thickness approaching the maximum for which surface stabilisation is effective. The computed properties model the optical properties of real cells accurately. Clearly the model has the potential to describe the dynamic properties of SSFLC cells also, though this would require that realistic values of the bulk and surface viscosities, η_o and η_s , were used. In the model the elastic energy associated with c-director and layer distortions has been considered but the coupling between them has been ignored. Also, the details of the relationships between the various chiral elastic constants were not considered. It would be interesting to investigate the role of these factors and to consider how a "chevron" layer structure might alter the director configuration. These factors could be investigated experimentally using dielectric measurements, phase retardation measurements and further conoscopic measurements.

7 Acknowledgements

I am indebted to Mr R.M.Sillitto, Dr D.G.Vass, Dr R.C.Dougal and other members of the Applied Optics group of the Department of Physics for helpful discussions. Thanks are also due to Mr P.Tuffy (physics), Dr J.E.Dixon (geology) and Mr J.Allan (University of St.Andrews, geology) for help in preparing the photographic results presented in this paper. Throughout this work Dr W.A.Crossland and Mr M.F.Bone (S.T.C. Technology Ltd.) have given both stimulus and encouragement and their company generously provided the LC cells used. Finally the award of an S.E.R.C. C.A.S.E. award with S.T.C. Technolgy Ltd. is gratefully acknowledged.

8 Appendix

The form of the Γ_i in equations (22) and (24) are:

$$\begin{aligned}
\Gamma_1 &= B_{13} \sin 2\psi \sin \phi - \cos^2 \psi (B_1 \sin^2 \phi + B_2 \cos^2 \phi) - B_3 \sin^2 \psi \\
\Gamma_2 &= \cos \psi \cos \phi (B_2 \sin \psi \sin \phi - C \cos \psi) \\
\Gamma_3 &= \frac{1}{2} B_{13} \sin 2\psi \cos \phi - \frac{1}{2} (B_1 - B_2) \cos^2 \psi \sin 2\phi \\
\Gamma_4 &= \cos \psi \cos \phi [\cos \psi \sin \phi (B_2 - A \cos 2\phi) + C \sin \psi (3 \sin^2 \phi + 1)] \\
\Gamma_5 &= \sin 2\psi (B_1 \sin^2 \phi + B_2 \cos^2 \phi - B_3) + 2B_{13} \cos 2\psi \sin \phi \\
\Gamma_6 &= -[D \cos \psi + D_1 \sin \psi \sin \phi + D_2 \cos \psi \cos 2\phi] \\
\Gamma_7 &= -P_s E \cos \psi \sin \phi + \epsilon_o \epsilon_\perp E^2 e [\sin \psi \cos \theta - \cos \psi \sin \phi \sin \theta] \cos \psi \cos \phi \sin \theta \\
\Gamma_8 &= \Gamma_1 \\
\Gamma_9 &= \Gamma_2 \\
\Gamma_{10} &= D_1 \cos \psi \sin \phi - D \sin \psi \\
\Gamma_{11} &= -2\gamma \sigma_2 (\sin \beta \cos \psi \cos \phi \sin \theta) \exp[-\gamma \sin^2 \beta] +
\end{aligned}$$

$$\begin{cases} \sigma_1 \gamma \sin \phi_1 \left(\frac{2\pi}{\pi + 2\phi_o} \right) \exp[-\gamma \sin^2 \left(\frac{\phi_1}{2} \right)] & \text{if } \phi \notin [2m\pi + \phi_o, (2m+1)\pi - \phi_o] \\ \sigma_1 \left(\frac{\pi}{\pi + 2\phi_o} \right) \sin 2\phi_2 & \text{otherwise} \end{cases}$$

The form of the Λ_i in equations (23) and (25) are:

$$\begin{aligned}
\Lambda_1 &= \frac{1}{2} C \sin 2\psi \sin 2\phi \cos \phi - B_2 \sin^2 \psi \sin^2 \phi - A \cos^2 \psi (1 - \sin^2 \phi \cos^2 \phi) \\
\Lambda_2 &= \cos \psi \cos \phi (B_2 \sin \psi \sin \phi - C \cos \psi) \\
\Lambda_3 &= \frac{1}{2} \sin 2\psi (B_3 - \sin^2 \phi (B_1 + B_2)) - B_{13} \cos 2\psi \sin \phi + C \cos^2 \psi \cos \phi \\
\Lambda_4 &= \frac{1}{2} A \sin 2\psi (1 - \sin^2 \phi \cos^2 \phi) - \frac{1}{2} B_2 \sin 2\psi \sin^2 \phi + C \sin \phi \cos^2 \phi (\cos^2 \psi - 2 \sin^2 \psi) \\
\Lambda_5 &= \frac{1}{2} A \cos^2 \psi \sin 4\phi + C \sin 2\psi \cos \phi (\cos^2 \phi - 2 \sin^2 \phi) - B_2 \sin^2 \psi \sin 2\phi \\
\Lambda_6 &= D \cos \psi + D_1 \sin \psi \sin \phi + D_2 \cos \psi \cos 2\phi \\
\Lambda_7 &= -P_s E \sin \psi \cos \phi + \frac{1}{2} \epsilon_o \epsilon_\perp E^2 e [\sin 2\psi (\sin^2 \phi \sin^2 \theta - \cos^2 \theta) + \cos 2\psi \sin \phi \sin 2\theta] \\
\Lambda_8 &= \Lambda_1 \\
\Lambda_9 &= \Lambda_2 \\
\Lambda_{10} &= \frac{1}{2} D_2 \cos \psi \sin 2\phi \\
\Lambda_{11} &= 2\gamma \sigma_2 \sin \beta (\cos \psi \cos \theta + \sin \psi \sin \phi \sin \theta) \exp[-\gamma \sin^2 \beta]
\end{aligned}$$

9 Tables

Material	Thickness
Liquid crystal (B.D.H. SCE3)	7 μm
Nylon	0.1 μm
ITO	0.05 μm
Glass	1 mm

Table 1: Specification of the LC cell

LC extraordinary refractive index, n_e	1.69
LC ordinary refractive index, n_o	1.50
Nylon refractive index, n_{nyl}	1.53
ITO refractive index, n_{ITO}	2.0
Glass refractive index, n_{gl}	1.54

Table 2: Optical constants used in the calculation

Spontaneous polarisation, P_s	88 $\mu C m^{-2}$
Cone angle, θ	25.5°
Parallel dielectric constant, $\epsilon_{ }$	3.10
Perpendicular dielectric constant, $\epsilon_{\perp}$	5.04

Table 3: Specification of the B.D.H. LC SCE3 at 15°C

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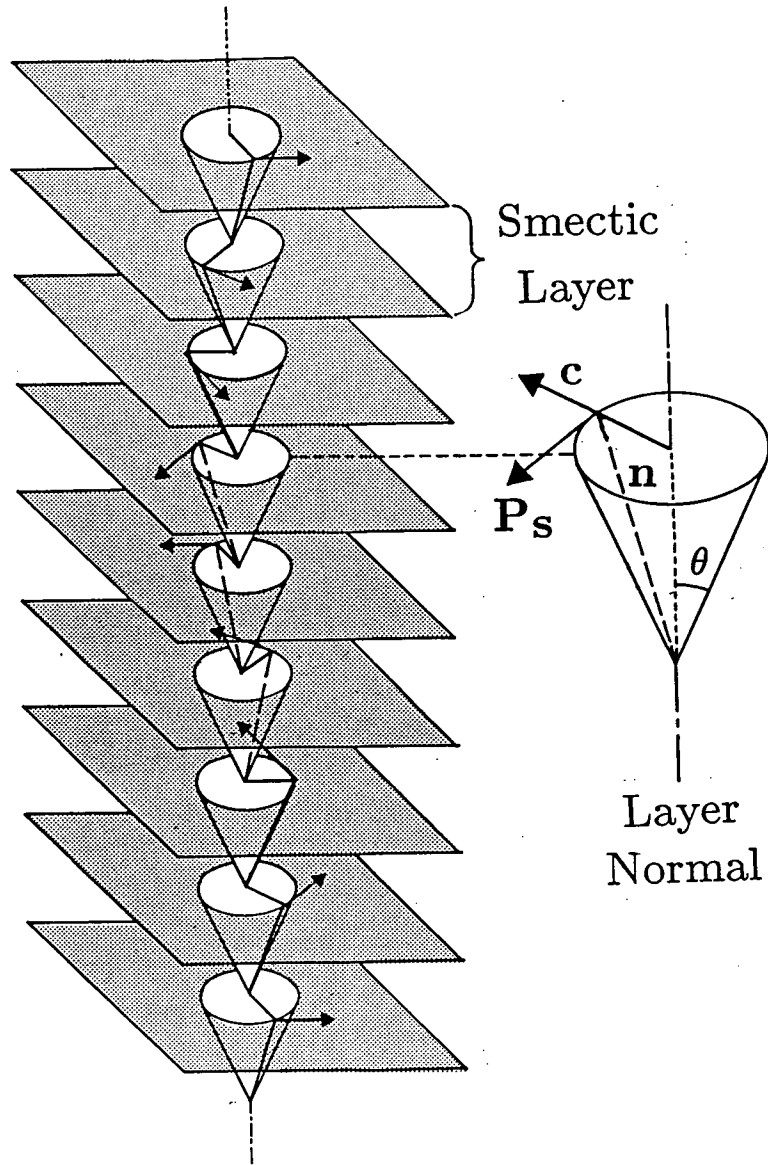


Figure 1: Director configuration in a bulk sample of SmC* LC. Within each smectic layer the $\mathbf{n}$ -director makes a constant angle θ with the layer normal and precesses about the layer normal from layer to layer. The spontaneous polarisation $\mathbf{P}_s$ lies in the smectic layer plane and perpendicular to the projection of the $\mathbf{n}$ -director onto the plane. This projected direction also defines the $\mathbf{c}$ -director orientation.

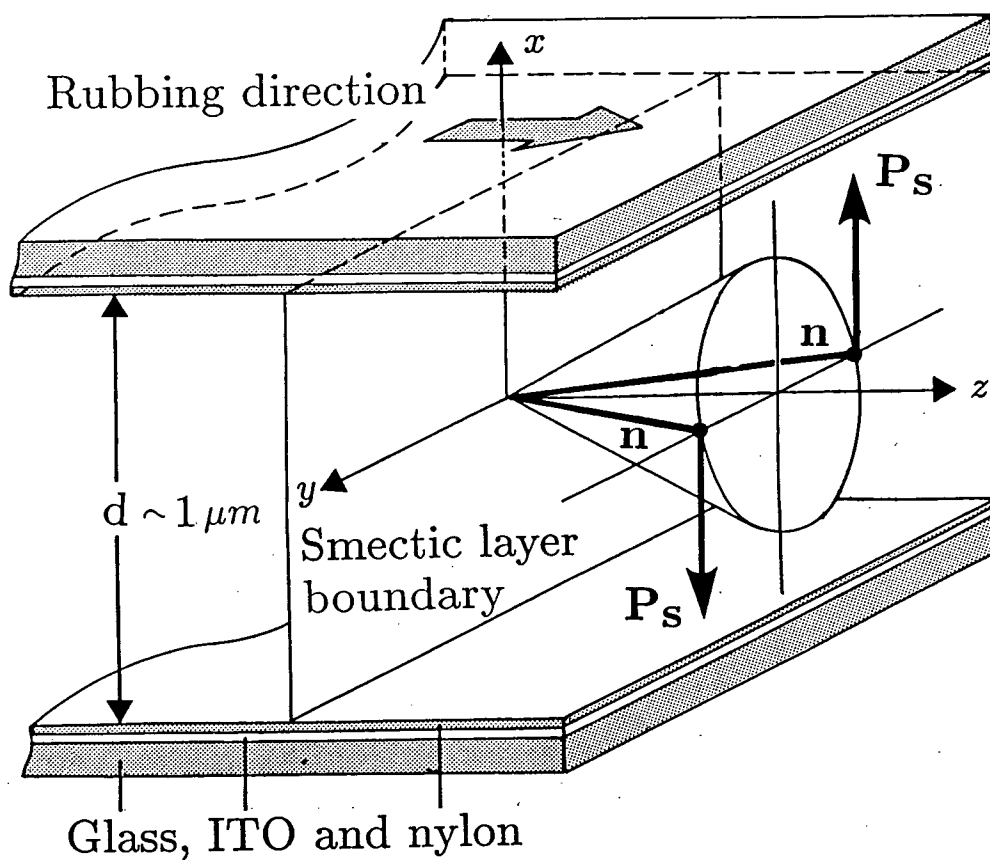


Figure 2: Ideal SSFLC cell. Provided that the cell thickness is small compared with the pitch length of the helix shown in figure 1 the helix is prevented from forming by surface forces. The $\mathbf{n}$ -director takes up one of the two stable orientations shown symmetrically positioned on either side of the rubbing direction. If a d.c. voltage is applied across the cell the $\mathbf{n}$ -director can be switched from one orientation to the other.

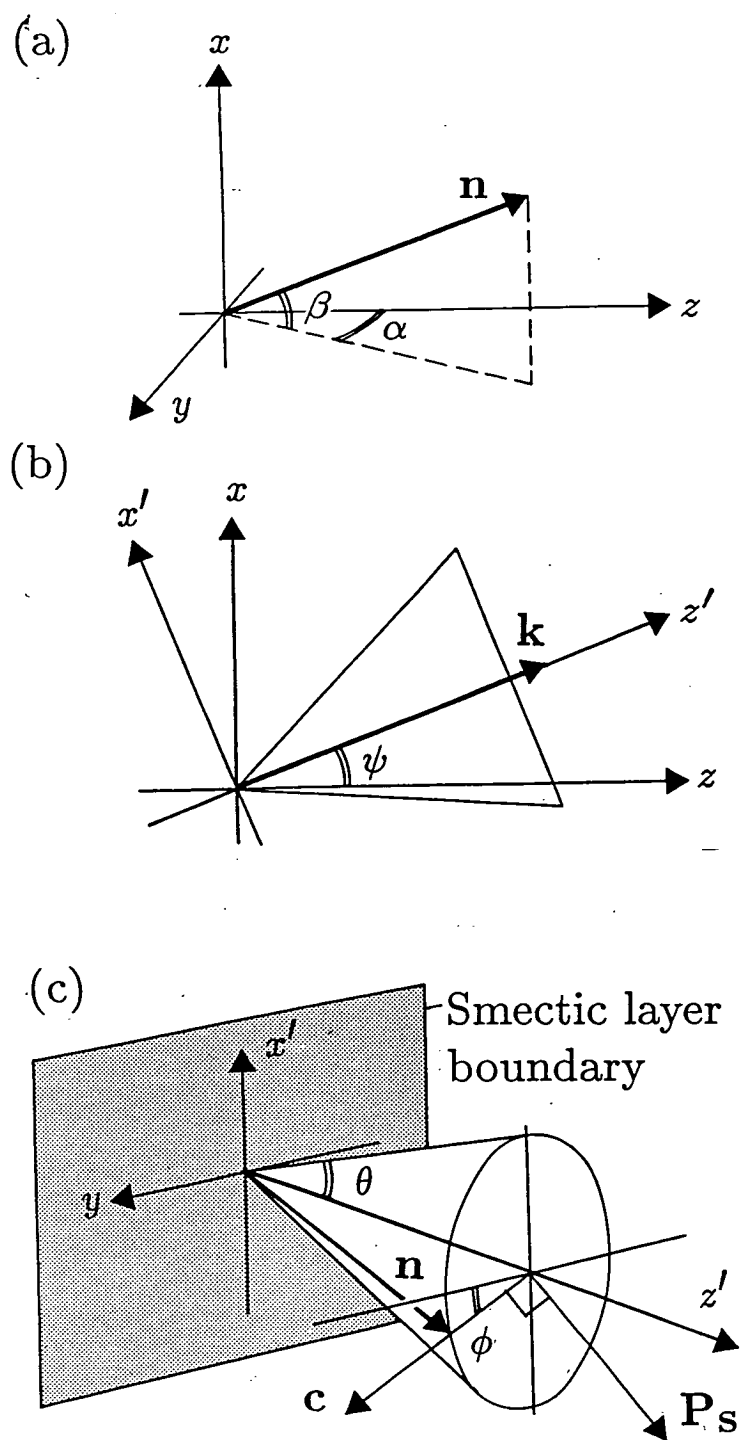


Figure 3: Coordinate system used in the theoretical formulation to describe the director orientation.

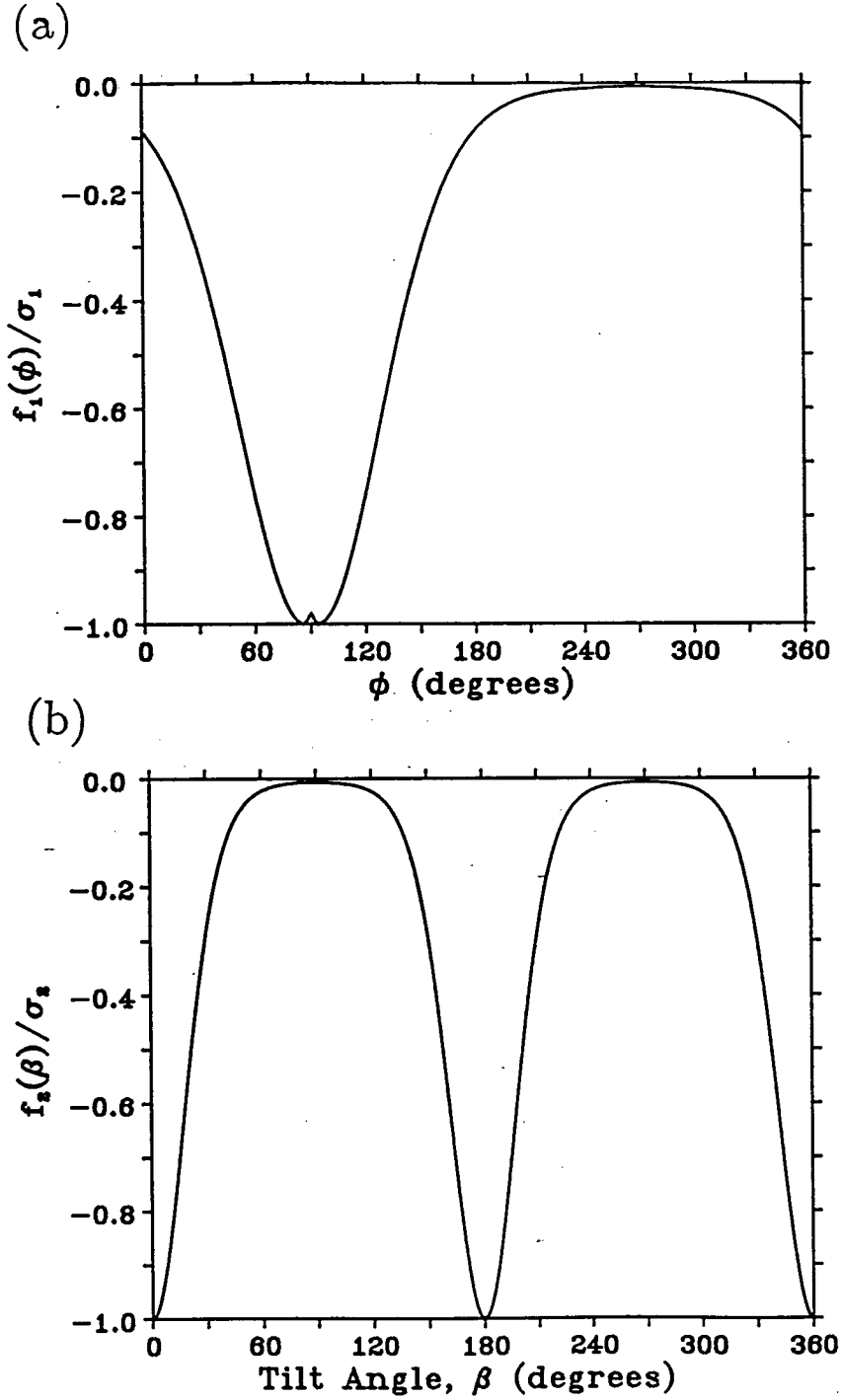


Figure 4: Form of the surface-interaction potentials a) $f_1(\phi)/\sigma_1$, and b) $f_2(\beta)/\sigma_2$, with $\gamma = 5$ and $\phi_o = 86.5^\circ$. γ controls the steepness of the potential wells and ϕ_o the controls positions of the minima in $f_1(\phi)$. The combined effect of the potentials is to produce uniformly tilted layers when no voltage is applied.

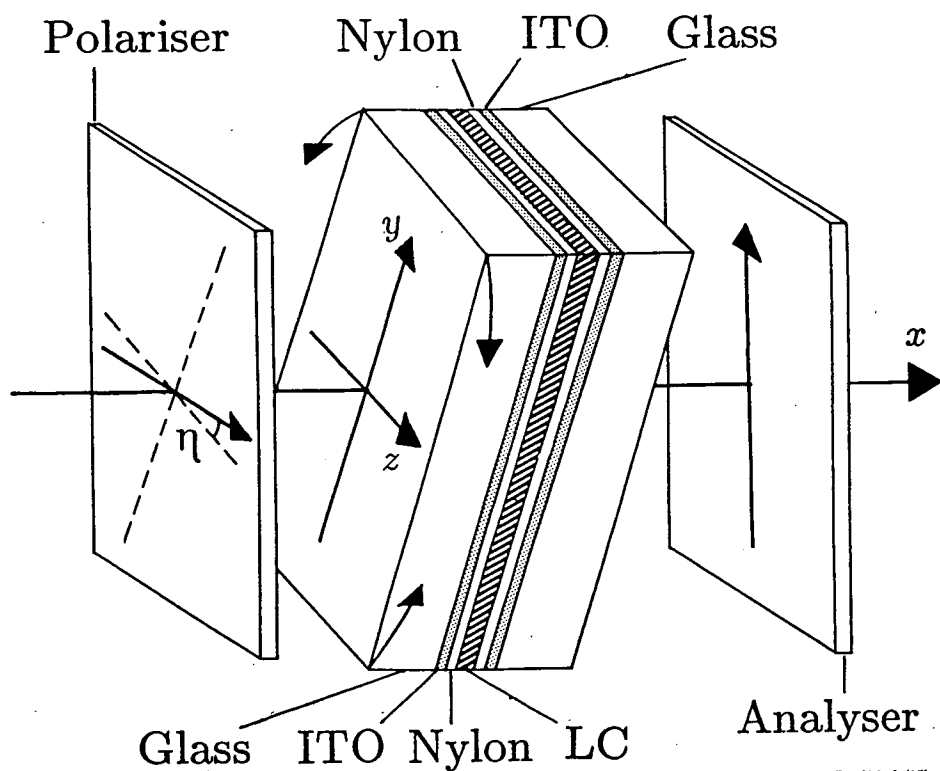


Figure 5: Model of the LC cell used in the optical calculations. The polariser and analyser were crossed and the LC cell was rotated about the x -axis to find the minimum transmission orientation. The rubbing direction is parallel to the z -axis and makes an angle η with the polariser axis.

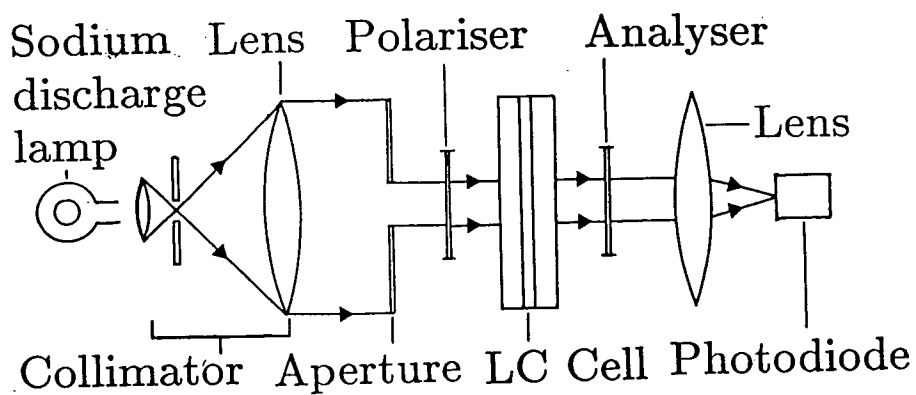


Figure 6: Schematic diagram of the optical bench used to measure the apparent azimuthal angle of the LC cell.

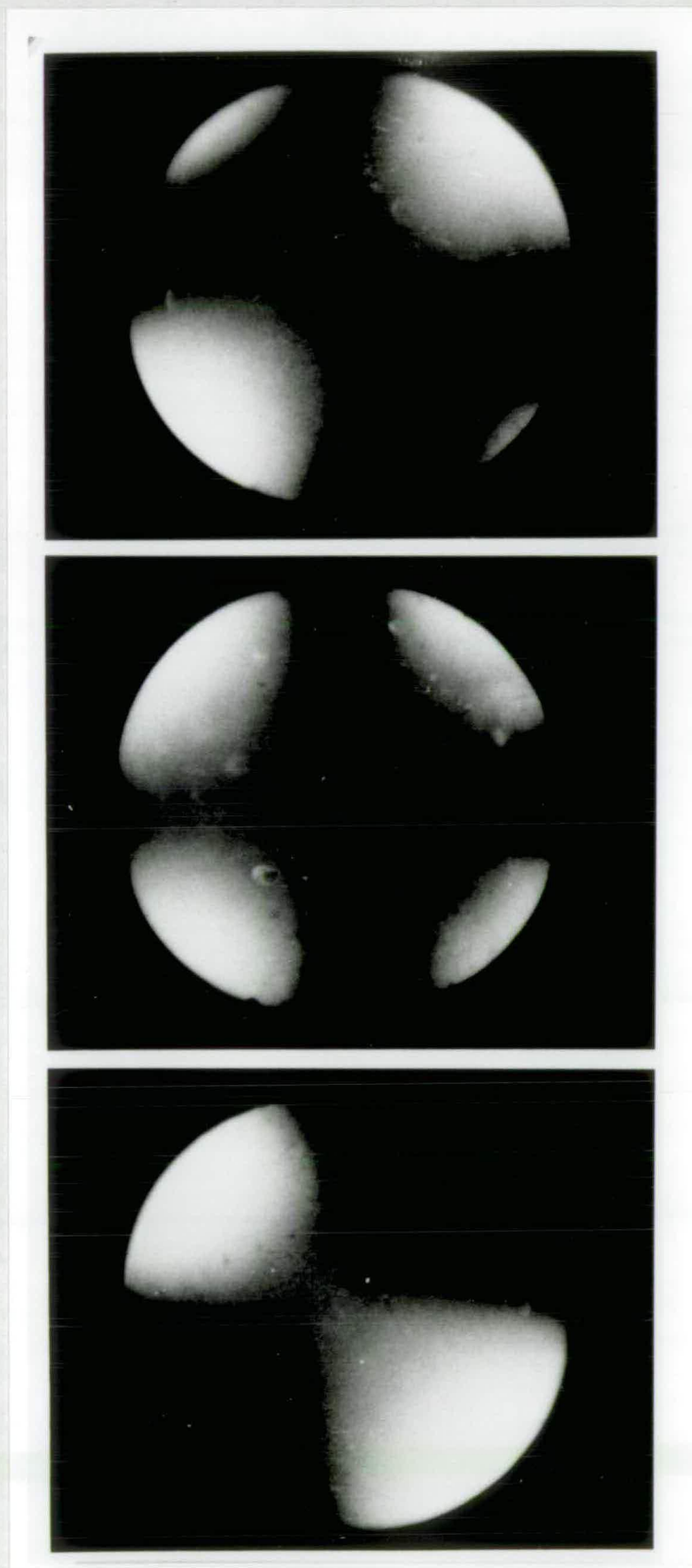


Figure 7: Conoscopic figures obtained for the LC SCE3 in a $7\mu\text{m}$ thick cell. The top and bottom images were obtained by rotating the cell approximately 1.5° away from the position in which the centre image was formed. The symmetric flash figure indicates that the mean orientation of the optic axis is in the cell plane.

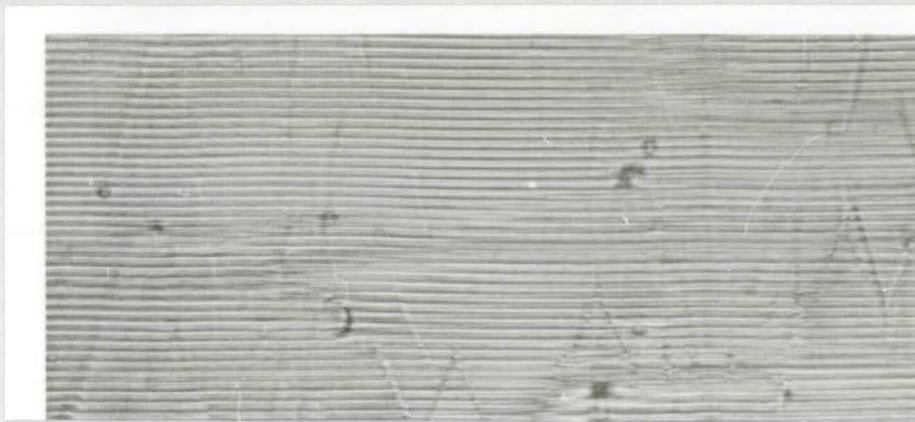


Figure 8: Dechiralisation lines exhibited by a $100\mu\text{m}$ thick LC cell containing SCE3 viewed in unpolarised light. These regularly spaced lines are linear discontinuities in the director orientation caused by the incompatibility of the orientations of the helical bulk director and the uniform surface director.

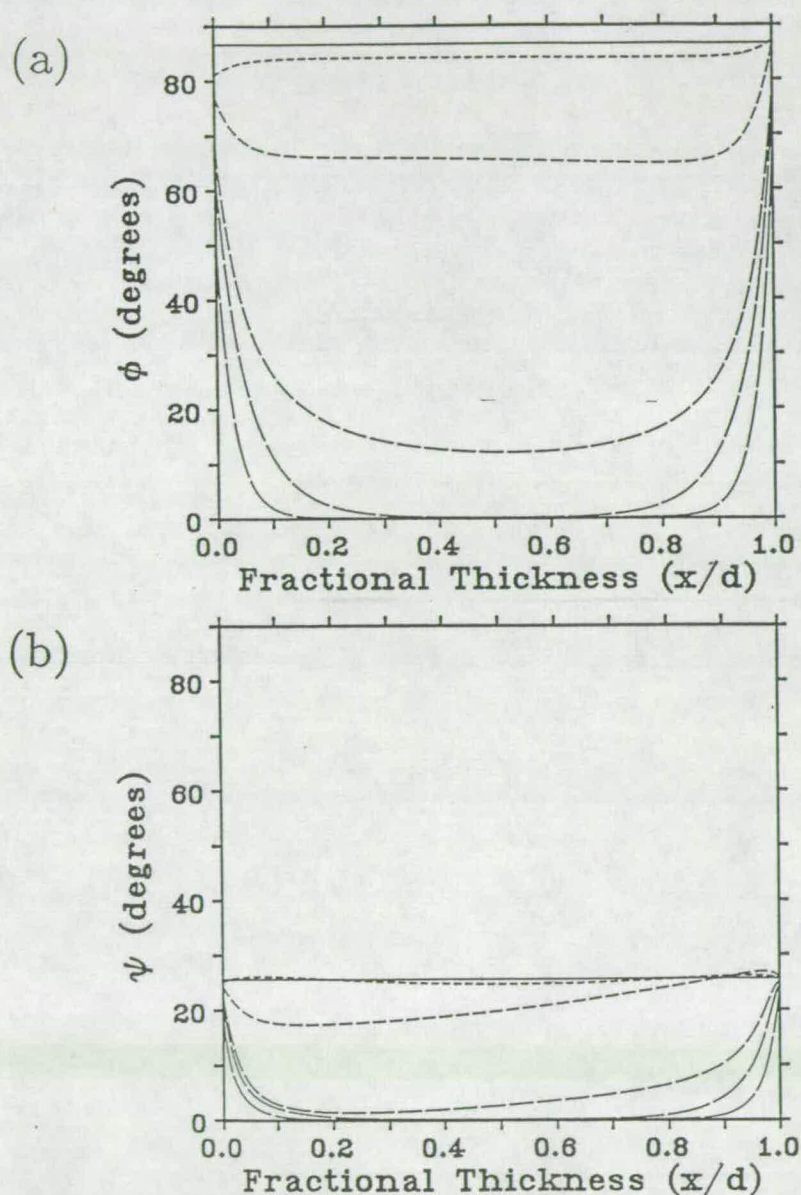


Figure 9: Computed variation of a) ϕ and b) ψ with fractional distance through the LC. The dotted curves and solid lines are the zero-voltage configurations with and without the chiral energy respectively. In order of increasing dash length the solid curves are the configurations including the chiral energy for applied voltages of 0.25V, 1V, 4V and 16V.

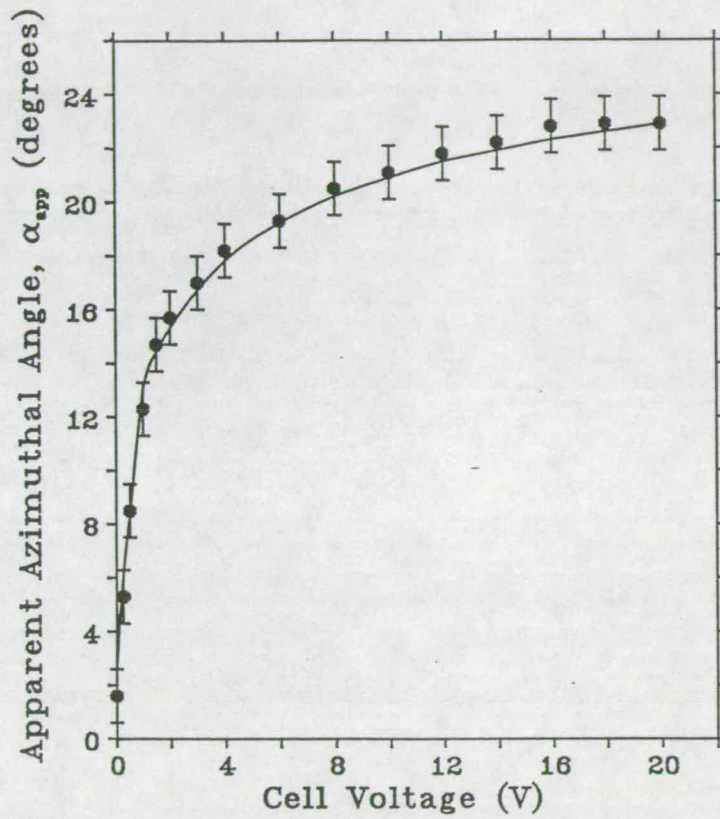


Figure 10: Variation of apparent azimuthal angle with cell voltage. The solid curve shows the computed points joined by a cubic spline and the points with the error bars represent the experimental measurements.

A Method for Computing Homogeneous-Liquid-Crystal Conoscopic Figures

Alastair R. MacGregor

Abstract

A model is presented for computing the conoscopic figures produced by a uniformly oriented liquid crystal (LC) in a thin cell observed with a polarising microscope. The method takes account of refraction and primary reflection at each interface within the cell but neglects multiple reflections. It is shown that the form of the isochromes in the figures is qualitatively given by the intersections of Bertin's surfaces with the LC surface but that refraction also influences the form of the isochromes. Examples of calculated conoscopic figures are presented including the "symmetric flash figure" and the optic-normal figure. The way in which these are altered by small changes in the optic-axis orientation is demonstrated. To complete the model the polarising effect of the microscope condenser and objective lens systems is estimated by calculating the Fresnel coefficients for model lens systems; the effect on the conoscopic figures is noted. Finally the director tilt in a $7\mu\text{m}$ chiral smectic C^* LC cell is determined by comparing an experimentally measured figure with a set of calculated figures.

1 Introduction

Conoscopic figures are usually observed with a polarising microscope. A parallel beam of light is passed in sequence through a polariser, a condenser lens system, an optically anisotropic sample, an objective lens system and an analyser which is crossed with respect to the polariser, and emerges as a parallel beam. The conoscopic figure is the interference pattern formed by the ordinary and extraordinary waves in the back focal plane of the objective lens system [1, chapter 9]. In a polarising microscope the Bertrand lens is inserted so that the figure may be viewed with the ocular lens system. When observed in white light the figure is composed of lines of equal colour (isochromes) and extinction positions (isogyres). If monochromatic light illuminates the sample then the isochromes constitute a pattern of dark and light fringes instead. Both isochromes and isogyres yield information about the orientation of the optic axis/axes. In particular, for a uniaxial sample the pattern of isochromes and isogyres, and the way in which this pattern moves when the sample is rotated, provides information about the angle at which the optic axis is tilted out of the plane of section.

Many nematic and smectic liquid crystals (LCs) are optically uniaxial or so weakly biaxial that they may be considered to be uniaxial for most purposes. In general LCs are optically inhomogeneous but uniform alignment of the optic axis, or director, is produced by appropriate surface-treatment of the cell [2, chapter 3]. When this treatment is used the conoscopic technique allows the director tilt to be measured. In this paper a method is presented for computing the conoscopic figures produced by such cells. The calculated figures are interpreted in terms of Bertin's surfaces (surfaces of constant phase difference between the ordinary and extraordinary waves) and the influence of the Fresnel coefficients on the figures is shown. Examples of calculated conoscopic figures are presented including the "symmetric flash figure" (zero tilt) and the optic-normal figure (90° tilt). The way in which these characteristic figures are altered by small orientational changes of the director is demonstrated. A model of the microscope condenser and objective lens systems is introduced to enable computation of the lens-induced polarisation. This effect is then incorporated into the conoscopic calculations and the effect on the figures is shown. Finally the experimental conoscopic figure for a $7\mu\text{m}$ thick chiral smectic C (SmC^*) LC is compared with the calculated figures and the director-tilt angle is determined.

2 Optical Description of a Homogeneous LC Cell

2.1 Light Propagation in a Uniaxial Medium

A variety of methods has been developed previously to investigate the propagation of light in a uniaxial layered medium [3,4] or [5, chapter 9.7]. These methods provide an exact solution to the problem and take account of refraction and multiple reflections between interfaces. However in the method described below multiple reflections were neglected as they usually have only a small effect on the transmitted electric field. This simplified treatment, based on that of Yeh [5, chapter 9.5–6], was found sufficient to describe all the experimentally observed phenomena associated with conoscopic figures and is much faster computationally than the exact methods. In this paper Yeh's method

is extended to allow any orientation of the director and to take account of isotropic layers on either side of the LC layer.

Consider a uniaxial plate of thickness d and refractive indices n_e and n_o positioned as shown in figure 1a. As shown in figure 1b the angles θ and ϕ define the tilt and twist of the director, $\mathbf{n}$. A plane wave with angular frequency ω and wave vector $\mathbf{K}$ is incident at angle χ , in the yz plane, on the front surface of the plate. At this surface the wave is divided into a reflected component, with wave vector $\mathbf{K}'$, and two transmitted components, the ordinary and extraordinary, with wave vectors $\mathbf{K}_o$ and $\mathbf{K}_e$. At the second surface the ordinary and extraordinary waves are reflected, with wave vectors $\mathbf{K}'_o$ and $\mathbf{K}'_e$, and transmitted, with wave vector $\mathbf{K}$.

At the first surface the incident, reflected and transmitted electric field vectors are

$$\mathbf{E}_i(z=0) = (A_s \hat{\mathbf{s}} + A_p \hat{\mathbf{p}}) \exp[i\omega t], \quad (1)$$

$$\mathbf{E}_r(z=0) = (B_s \hat{\mathbf{s}} + B_p \hat{\mathbf{p}}') \exp[i\omega t], \quad (2)$$

$$\mathbf{E}_t(z=0) = (C_o \hat{\mathbf{o}} + C_e \hat{\mathbf{e}}) \exp[i\omega t], \quad (3)$$

where $\hat{\mathbf{s}}$ is a unit vector perpendicular to the plane of incidence and is given by $\hat{\mathbf{s}} = \mathbf{x}$ as shown in figure 1a. $\hat{\mathbf{p}}$ and $\hat{\mathbf{p}}'$ are unit vectors parallel to the plane of incidence and are given by

$$\hat{\mathbf{p}} = \mathbf{K} \times \hat{\mathbf{s}} / |\mathbf{K}|, \quad (4)$$

$$\hat{\mathbf{p}}' = \mathbf{K}' \times \hat{\mathbf{s}} / |\mathbf{K}'|. \quad (5)$$

$\hat{\mathbf{o}}$ and $\hat{\mathbf{e}}$ are unit vectors parallel to the electric field vectors of the ordinary and extraordinary waves in the uniaxial medium.

At the first surface the tangential components of the wave vectors, β , are equal so we may write

$$\mathbf{K} = \beta \mathbf{y} + K_z \mathbf{z}, \quad (6)$$

$$\mathbf{K}' = \beta \mathbf{y} - K_z \mathbf{z}, \quad (7)$$

$$\mathbf{K}_o = \beta \mathbf{y} + K_{oz} \mathbf{z}, \quad (8)$$

$$\mathbf{K}_e = \beta \mathbf{y} + K_{ez} \mathbf{z}. \quad (9)$$

Let n be the refractive index of the surrounding medium so that

$$\beta = (\omega/c)n \sin \chi \quad (10)$$

and K_z , the z -component of $\mathbf{K}$, is given by

$$K_z = (\omega/c)n \cos \chi. \quad (11)$$

Expressions for the z -components of $\mathbf{K}_o$ and $\mathbf{K}_e$, K_{oz} and K_{ez} , are given in appendix A. The ordinary and extraordinary refraction angles, χ_o and χ_e , are found using equations 8 and 9:

$$\chi_o = \arctan(\beta/K_{oz}), \quad (12)$$

$$\chi_e = \arctan(\beta/K_{ez}). \quad (13)$$

The ordinary and extraordinary refractive indices are n_o and $n_e(\chi_e)$ where

$$n_e(\chi_e) = \frac{K_{ez}}{(\omega/c) \cos \chi_e}. \quad (14)$$

The unit vectors $\hat{o}$ and $\hat{e}$ are (appendix B):

$$\hat{o} = N_o \mathcal{M}(-\beta \cos \phi, \beta \sin \theta \sin \phi - K_{oz} \cos \theta, 0)^T, \quad (15)$$

$$\hat{e} = N_e \mathcal{M} \left(\frac{K_{ez} \cos \theta - \beta \sin \theta \sin \phi}{n_e^2(\chi_e) - n_o^2}, \frac{-\beta \cos \phi}{n_e^2(\chi_e) - n_o^2}, \frac{K_{ez} \sin \theta + \beta \cos \theta \sin \phi}{n_e^2(\chi_e) - n_e^2} \right)^T, \quad (16)$$

where N_o and N_e are normalising constants, $\mathcal{M}$ is the rotation matrix given in appendix A relating the components of a vector in the dielectric ellipsoid frame of reference to those in the xyz frame. Since we have defined the electric field vectors fully the magnetic field vectors can be derived from Maxwell's equations. As Yeh [5, chapter 9.6] shows, the continuity of the tangential components of the electric and magnetic field vectors leads to equations for the ordinary and extraordinary electric field amplitudes C_o and C_e . His equations 9.6–28 and 9.6–29 may be used directly by replacing his expressions for the wave vectors and field vectors by the more general expressions derived in this paper.

At the second surface the incident, reflected and transmitted electric field vectors are

$$\mathbf{E}_i(z=d) = (C_o \hat{o} \exp[-iK_{oz}d] + C_e \hat{e} \exp[-iK_{ez}d]) \exp[i\omega t], \quad (17)$$

$$\mathbf{E}_r(z=d) = (C'_o \hat{o}' + C'_e \hat{e}') \exp[i\omega t], \quad (18)$$

$$\mathbf{E}_t(z=d) = (A'_o \hat{s} + A'_p \hat{p}) \exp[i\omega t], \quad (19)$$

where $\hat{o}'$ and $\hat{e}'$ are unit vectors parallel to the electric field vectors of the reflected ordinary and extraordinary waves, C'_o and C'_e are their complex amplitudes and A'_o and A'_p are the complex amplitudes of the transmitted electric field vectors. At the second surface the tangential components of the wave vectors are equal so we may write

$$\mathbf{K}'_o = \beta \mathbf{y} + K'_{oz} \mathbf{z}, \quad (20)$$

$$\mathbf{K}'_e = \beta \mathbf{y} + K'_{ez} \mathbf{z}. \quad (21)$$

Expressions for the z -components of $\mathbf{K}'_o$ and $\mathbf{K}'_e$, K'_{oz} and K'_{ez} , are given in appendix A. The refraction angles χ'_o and χ'_e , the refractive index $n_e(\chi'_e)$ and the unit vectors $\hat{o}'$ and $\hat{e}'$ are determined from equations 12 to 16 by replacing the (unprimed) variables describing the forward-propagating waves with the (primed) variables describing the backward-propagating waves. As at the front surface, the magnetic field vectors may be written down in terms of the electric field vectors. The continuity of the tangential components of the electric and magnetic field vectors is then expressed as a set of four simultaneous equations. These are solved for the complex amplitudes C'_o , C'_e , A'_o and A'_p . If we ignore multiple reflections then the amplitudes of the transmitted waves are simply given by A'_o and A'_p .

2.2 Light Propagation in an Isotropic Medium

The method described above must be augmented to take account of isotropic layers if a complete LC cell, shown schematically in figure 2, is to be modelled. On each

side of the LC is a nylon alignment layer which produces uniform alignment of the LC molecules, a transparent conductive coating (indium tin oxide) and a layer of glass. At each interface the amplitude transmission and reflection coefficients are described by Fresnel's equations. Consider an interface between two isotropic media of refractive indices n_1 and n_2 . A plane wave is incident at angle χ_1 to the interface normal. If the electric field components parallel and perpendicular to the plane of incidence are E_p and E_s , then the transmitted components T_p and T_s are given [6, chapter 1.5] by

$$T_p = E_p \left(\frac{2n_1 \cos \chi_1}{n_2 \cos \chi_1 + n_1 \cos \chi_2} \right), \quad (22)$$

$$T_s = E_s \left(\frac{2n_1 \cos \chi_1}{n_1 \cos \chi_1 + n_2 \cos \chi_2} \right), \quad (23)$$

where χ_2 is the direction of propagation of the transmitted wave and is related to χ_1 by Snell's law. These equations are used to describe the transmission at each interface between isotropic media in the LC cell. The amplitudes A_s and A_p are modulated at each interface before the light reaches the LC layer and the amplitudes A'_s and A'_p at each interface after the LC layer.

3 Simulation of Conoscopic Figures

We now apply the optical method outlined in section two to the calculation of the conoscopic figures produced by a cell containing homogeneously aligned LC. It will be assumed that the polariser and (crossed) analyser are perfect polarisers for normally incident light and that the condenser and objective lens systems are free from spherical and other aberrations for the monochromatic light used. Figure 3 shows the coordinate systems used in the conoscopic calculations. In the simulation r_{max} is the lens radius and the radius of the field-of-view and χ_{max} is the maximum angle of incidence to the LC cell. The complete optical system is fixed in space in the $x'y'z$ coordinate system and the xyz coordinate system is related to it by the angle ρ . The x' -axis is the polariser axis and y' -axis is the analyser axis. In the $x'y'z$ system the projection of the LC director onto the $x'y'$ plane makes an angle of ϕ' with the x' axis. Therefore in the xyz system the angle ϕ is given by $\phi' - \rho$. Light passing through the polariser at point P at radius r will pass through the analyser at point Q . The angle of incidence χ is given by

$$\tan \chi = \frac{r \tan \chi_{max}}{r_{max}}. \quad (24)$$

If the amplitude of the electric field vector of the light transmitted by the polariser is E then, neglecting the Fresnel coefficients of the lenses as a first approximation, after passing through the lens

$$A_s = E \cos \rho, \quad (25)$$

$$A_p = -E \sin \rho. \quad (26)$$

The method of section two is then applied to calculate the complex amplitudes A'_s and A'_p transmitted by the LC cell. After passing through the objective lens system and the analyser the complex amplitude transmittance T is given by

$$T = A'_s \sin \rho + A'_p \cos \rho \quad (27)$$

and the intensity transmittance is given by the square modulus of T . The conoscopic image is built up by calculating the intensity transmittance at each point on a square grid within a circle of radius r_{max} .

Although the lens-induced polarisation normally plays only a minor role in determining the form of the conoscopic figure (cf section 4.3) there are circumstances in which the effect is important. In particular, if the uniaxial medium produces a small phase difference between the ordinary and extraordinary waves the conoscopic figure may be dominated by the effect of the lenses. To take account of this possibility the Fresnel coefficients of the microscope lenses were estimated by modelling each with the lens triplet shown in figure 4. It was designed to be free from spherical aberration and to refract the light by a similar amount at each lens. Lens 1 in the triplet is a sphero-ellipsoid [7, chapter 5] and transforms a plane wave incident on the ellipsoidal surface into a spherical wave converging towards the second focus of the ellipsoid. Lenses 2 and 3 are aplanats [8, chapter 5] which decrease the radius of curvature of the wavefront. In each of the three lenses the radius of curvature of the back surface is matched to the wavefront curvature.

First we consider the condenser lens system shown in figure 4. The Fresnel coefficients for the lens when $\chi = \chi_3$ were calculated as follows. Let θ_{il} and θ_{tl} be the angles of incidence and transmission at the front surface of lens l and let χ_l be the angle which the transmitted ray makes with the z -axis. It can be shown [8, chapter 5] that for the aplanatic lens 3, $\theta_{i3} = \chi_3$ and $\theta_{t3} = \chi_2$, so that Snell's law may be written as

$$\chi_2 = \arcsin \left(\frac{n \sin \chi_3}{n_{gl}} \right), \quad (28)$$

where n_{gl} is the refractive index of the lens. From these relationships the Fresnel coefficients (equations 22 and 23) for the lens may be calculated. In the same way the coefficients for lens 2 may then be calculated. At the front surface of lens 1 $\theta_{i1} = \theta_{t1} + \chi_1$. Substituting this relationship into Snell's law and rearranging we obtain

$$\theta_{t1} = \arctan \left(\frac{n \sin \chi_1}{n_{gl} - n \cos \chi_1} \right). \quad (29)$$

Therefore the Fresnel coefficients for lens 1 may be calculated, along with the coefficients for the complete condenser triplet, by multiplying together the coefficients for each component. The objective lens system was modelled by reversing the condenser triplet described above and calculating the Fresnel coefficients in the same way.

4 Interpretation of Conoscopic Figures

4.1 Bertin's Surfaces

As noted in section 1 conoscopic figures may be described in terms of two components: isochromes and isogyres. Isochromes are contour lines joining parts of the figure which have the same phase difference between ordinary and extraordinary waves. In polychromatic light isochromes appear as lines of equal colour and in monochromatic light as lines of equal fringe brightness. Isogyres are the extinction positions in the figure which correspond to optical paths for which only ordinary or only extraordinary waves are

excited. When the LC cell is rotated about the z -axis the isochromes rotate with the cell whereas the isogyres either remain stationary or move relative to the isochromes in a way that depends on the director-tilt angle.

If we temporarily ignore the refraction which occurs at the LC surfaces the shape of the isochromes can be understood by considering Bertin's surfaces. Figure 5 shows the centre sections of Bertin's surfaces in a uniaxial medium for phase differences of one, two and three wavelengths. The surfaces indicate the distance that light must travel from the point O in any direction to produce a specified phase difference between the ordinary and extraordinary waves. Normal to the optic axis the surfaces are circular in cross-section. Within a slab of uniaxial material of thickness d the positions of the isochromes are determined (if refraction is neglected) by the intersections of Bertin's surfaces with the plane $z = d$. In general the phase difference introduced between the ordinary and extraordinary waves, Δ , is given by

$$\Delta = (K_{ez} - K_{oz})d. \quad (30)$$

If the phase difference is an integral number of wavelengths extinction occurs but if the phase difference is an odd number of half-wavelengths the transmittance is maximised. When the uniaxial material is rotated about the z -axis the pattern of isochromes rotates with it and is thus distinct from the pattern of isogyres. In fact the positions of the isochromes are altered somewhat from the positions described above by refraction at the LC interfaces. However the Bertin's surfaces still provide a good qualitative explanation of the form of the isochromes.

4.2 Characteristic Conoscopic Figures

There are certain director-orientations which give characteristic conoscopic figures. These are illustrated in the following examples where the data given in table 1 is used in the model of sections 2 and 3 to describe the LC cell shown schematically in figure 2. The LC refractive indices used are for the SmC* liquid crystal SCE3 (B.D.H. Limited). In each example the transmitted intensities were calculated for a circular field-of-view with 256 values plotted across the diameter. The contrast of the resulting image was then enhanced using histogram equalisation [9] to emphasise the form and symmetry of the pattern. Experimentally the image enhancement was carried out photographically by pushing the contrast during development and printing but could equally well have been done using an array camera, frame-grabber and histogram equalisation. So far the polarising effect of the lenses has been ignored but will be considered in section 4.3.

4.2.1 Symmetric/Uniaxial Flash Figure

The conoscopic figures produced by rotating the sample about the z -axis when the director is in the plane of the LC cell ($\theta = 0$) are collectively called the symmetric or uniaxial flash figure [10, chapter 7] on account of the rapid appearance and disappearance of the isogyres. When the director is aligned with the polariser axis ($\phi' = 0$) the isogyres form a dark symmetric cross as shown in figure 6a. As the sample is rotated away from this position in either direction the cross breaks up into two hyperbolic isogyres which separate rapidly (figure 6b) and leave the field-of-view in the quadrants containing the optic axis. In this configuration the orientations of Bertin's surfaces are

shown in figure 6c. Only the 2λ -surface (where λ is the wavelength of the illuminating light) intersects the LC surface within the field-of-view and it is this which causes the broadening of the vertical arms of the isogyres. However the isochrome is very indistinct for two reasons: refraction at the LC surface rotates the polarisation away from the director; and because the Bertin's surface crosses the LC surface at a small angle which reduces the fringe contrast. The effect of the refraction can be seen by noting the way in which the polarisation is rotated if an isotropic slab replaces the LC cell as shown in figure 6d. Rotation away from the x' -axis is exaggerated by a factor of four in this plot.

If the tilt angle is set at 5° , as shown in figure 7, the isochrome is much more easily visible and remains so as it rotates with the sample. In comparison with the symmetric flash figure the symmetry of the isogyres is clearly altered and this enables the small change in director-orientation to be detected. As the director tilt is increased the symmetric cross is further distorted and the contrast of the isochromes increases as the Bertin's surface is intersected by the LC surface at larger angles.

4.2.2 Optic-Normal Figure

The optic-normal conoscopic figure [10, chapter 7] is produced when the director is normal to the plane of the LC ($\theta = 90^\circ$). As shown in figure 8a the isogyres form a dark cross centered on the optic axis which, unlike the cross of the uniaxial flash figure, remains unchanged when the sample is rotated. Figure 8b shows the orientation of Bertin's surfaces and the reason why no isochromes are visible. If the optic axis is tilted away from the normal position by 5° (i.e. $\theta = 85^\circ$) the cross centre follows it across the field-of-view as shown in figure 9a. When the LC cell is rotated the centre of the cross again follows the optic axis but the orientation of the cross remains unchanged (figure 9b).

4.2.3 Intermediate Figures

Conoscopic figures for tilt angles of 10° to 80° are shown in figure 10. As the tilt angle increases the 2λ -isochrome moves down the field of view, the 1λ -isochrome enters the field of view followed by the optic axis and finally the 2λ -isochrome leaves the foot of the field-of-view.

4.3 Lens-Induced Polarisation

In all of the above calculations the polarising effect of the microscope condenser and objective lenses was ignored. However the effect can be modelled, as described in section 3, and included in the calculation of the conoscopic figures. A refractive index of 1.519, that of the low-dispersion glass BK7, was assumed. The polarising effect of the lenses is most easily seen when the LC cell is removed altogether and the "isotropic cross" [11] is formed. It is shown in figure 11 along with a plot showing the polarisation-rotation produced by a pair of the triplet lenses described in section 3. In the polarisation plot each line represents the polarisation direction after passing through the lenses. The deviation from the vertical has been exaggerated by a factor of four for the sake of clarity. Figures 11c and d show two conoscopic figures calculated when the lens-induced polarisation was taken into account. Most obvious is the effect on the isochrome which

is completely eliminated in figure 11c. By contrast the isogyre positions are largely maintained though their shape is altered. The alteration in the figures caused by the lens-induced polarisation is concluded to be of importance if quantitative measurements are to be made on real conoscopic figures.

5 Conoscopic Measurements

In a SmC* liquid crystal the molecules form a layered structure and tilt away from the layer normal by a constant angle (typically $20 - 25^\circ$) [12]. Within each layer the molecular orientation has a well-defined mean, the director, which at optical frequencies coincides with the uniaxial optic axis [13]. The molecules' transverse dipoles are aligned perpendicular to the director and to the layer normal so that there is a spontaneous polarisation within each layer. As a result of the chirality of the SmC* LC molecules the director and the spontaneous polarisation precess from layer to layer along the layer normal with a helical pitch of order $10\mu\text{m}$. However when the LC is confined between polymer-coated glass plates with a separation less than the helical pitch the helical structure is unable to form and the LC is optically uniform and ferroelectric. The rôle of the polymer coating is to produce director alignment parallel to the surfaces as in nematic LC devices [2, chapter 3]. Confined in this way the LC director configuration through the cell is uniform to within a couple of degrees [12] and occupies one of two stable states. In one the spontaneous polarisation is pointing partially upwards and in the other partially downwards. Switching between the two states is accomplished by applying a voltage across transparent conducting layers of indium tin oxide (ITO) sandwiched between the polymer and glass layers of the cell. The switching process occurs rapidly ($< 100\mu\text{s}$) because of the strong coupling between the electric field and the spontaneous polarisation.

A $7\mu\text{m}$ cell containing the SmC* liquid crystal SCE3 (B.D.H. Limited) was supplied by S.T.C. Technology Limited with nylon alignment layers, a microscope slide as the bottom surface of the cell and a microscope cover-slip as the top surface. This allowed conoscopic examination using microscope objectives with working distances as short as 0.1mm . No ITO coatings were included as only the zero-field conoscopic figures were required. Photographs were taken with a camera mounted on a Leitz Ortholux 2 Pol.-Ek. polarising microscope fitted with a $50\times$ objective lens of numerical aperture 0.85 (equivalent to a cone angle $\chi = 58.2^\circ$) and a white light source. Figure 12a shows the zero-twist ($\phi' = 0$) conoscopic figure produced by the cell described above. In this photograph the isogyre was made more distinct by increasing the contrast during the film development and printing. The figure indicates, by the asymmetry of the cross, that there must be a small director-tilt in the cell. A set of conoscopic figures was calculated, using the data in table 1, for tilt angles of 0 to 5° in 1° steps and a cone angle of 58.2° . By comparing these figures with figure 12a the director tilt angle was found to be $2^\circ \pm 1^\circ$ in good agreement with calculated director structures [12]. Figure 12b and c show the calculated conoscopic figures with (b) and without (c) histogram equalisation for $\theta = 2^\circ$. Theoretical and experimental figures appear rather different because of the different image-processing techniques employed but in both cases the isogyre positions are clearly visible.

6 Conclusions

The model presented in this paper allows rapid and realistic computation of conoscopic figures produced by cells containing homogeneously aligned LC. Image enhancement of the calculated figures shows the location of the isochromes and isogyres precisely although they would normally be indistinct for a sample of the thickness commonly used in LC cells. Comparison of the figures with the intersections of the LC surface and Bertin's surfaces shows the importance of refraction in determining conoscopic figures. Through the introduction of a model of the microscope condenser and objective lens systems the degree of lens-induced polarisation is estimated and this effect is included in the conoscopic calculations. The practical use of the model is demonstrated by its application to a $7\mu\text{m}$ thick cell containing the SmC* liquid crystal SCE3. The director tilt is determined by comparing the isogyre position in the experimentally measured conoscopic figure with the positions in the calculated figures. In this way the conoscopic technique may be used quantitatively for any director-orientation. A useful extension of this work would be to calculate the conoscopic figures produced by non-uniform director structures using one of the methods referred to in section 2.1. This would provide a useful check on the form of any calculated director structures.

7 Acknowledgements

I am indebted to Mr R.M.Sillitto, Dr D.G.Vass, Dr R.C.Dougal and other members of the Applied Optics Group of the Department of Physics for helpful discussions and to Dr W.A.Crossland of S.T.C. Technology Ltd. for advice, encouragement and the supply of the LC cell used. Thanks are also due to Mr P.Tuffy (Physics) and Mr J.Allan (University of St.Andrews, Geology) for help with photography and to Mr J.M.Murison (Edinburgh University Computing Service) for help with the grey-scale plots. Finally the award of an S.E.R.C. C.A.S.E. award in collaboration with S.T.C. Technology Ltd. is gratefully acknowledged.

8 Appendix A: Derivation of the Wave Vectors

Consider a general anisotropic dielectric medium with principal dielectric tensor components ϵ_a, ϵ_b and ϵ_c subtending Euler angles θ^*, ϕ^* and ψ^* with respect to the xyz coordinate system [14, chapter 4]. In a uniaxial medium $\epsilon_a = \epsilon_b$ so the angle ψ^* may be chosen arbitrarily. Let us define $\theta = 90^\circ - \theta^*$ and $\phi = \phi^* - 90^\circ$ as in figure 1 and set $\psi^* = 90^\circ$. The rotation matrix which relates the components of a vector in the dielectric ellipsoid frame to those in the xyz reference frame is then [14, chapter 4]:

$$\mathcal{M} = \begin{pmatrix} -\sin \theta \cos \phi & \sin \phi & \cos \theta \cos \phi \\ -\sin \theta \sin \phi & -\cos \phi & \cos \theta \sin \phi \\ \cos \theta & 0 & \sin \theta \end{pmatrix}. \quad (31)$$

This matrix relates two orthogonal coordinate systems, so $\mathcal{M}^{-1} = \mathcal{M}^T$. In the dielectric ellipsoid frame of reference the ordinary and extraordinary wave vectors are

$$(\mathbf{K}_o)_{ell} = \mathcal{M}^T \mathbf{K}_o = (K_{ox} \cos \theta - \beta \sin \theta \sin \phi, -\beta \cos \phi, K_{oz} \sin \theta + \beta \cos \theta \sin \phi)^T, \quad (32)$$

$$(\mathbf{K}_e)_{ell} = \mathcal{M}^T \mathbf{K}_e = (K_{ex} \cos \theta - \beta \sin \theta \sin \phi, -\beta \cos \phi, K_{ez} \sin \theta + \beta \cos \theta \sin \phi)^T. \quad (33)$$

Maxwell's equations require [5, chapter 9.5] that $(\mathbf{K}_o)_{ell}$ and $(\mathbf{K}_e)_{ell}$ satisfy

$$\frac{K_o^2}{n_o^2} = \frac{\omega^2}{c^2}, \quad (34)$$

$$\frac{K_{ea}^2 + K_{eb}^2}{n_e^2} + \frac{K_{ec}^2}{n_o^2} = \frac{\omega^2}{c^2}, \quad (35)$$

where $K_o = |(\mathbf{K}_o)_{ell}|$ and K_{ea}, K_{eb} and K_{ec} are the components of $(\mathbf{K}_e)_{ell}$ along the axes of the dielectric ellipsoid. Substituting 32 into 34 we obtain the two solutions

$$K_{oz} = \pm \sqrt{\left(\frac{n_o \omega}{c}\right)^2 - \beta^2}, \quad (36)$$

the positive and negative corresponding to the z -components of the forward and backward propagating ordinary waves, K_{oz} and K'_{oz} , respectively. Substituting 33 into 35 we obtain, after rearrangement, the two solutions

$$K_{ez} = -\beta \frac{\epsilon_{13}}{\epsilon_{33}} \pm \frac{(\epsilon_{||}\epsilon_{\perp})^{\frac{1}{2}}}{\epsilon_{33}} \sqrt{\epsilon_{33} \left(\frac{\omega}{c}\right)^2 - \beta^2 \left(1 - \frac{\Delta\epsilon}{\epsilon_{||}} \cos^2 \theta \cos^2 \phi\right)} \quad (37)$$

where

$$\begin{aligned} \epsilon_{13} &= \Delta\epsilon \sin \theta \cos \theta \sin \phi, \\ \epsilon_{33} &= \epsilon_{\perp} + \Delta\epsilon \sin^2 \theta, \\ \Delta\epsilon &= \epsilon_{||} - \epsilon_{\perp}, \\ \epsilon_{||} &= n_e^2, \\ \epsilon_{\perp} &= n_o^2. \end{aligned}$$

When the positive and negative roots are taken, the solutions correspond to the z -components of the forward and backward propagating extraordinary waves, K_{ez} and K'_{ez} , respectively.

9 Appendix B: Derivation of the Electric Vector Directions

Let us define the vectors $\hat{\mathbf{s}}_o$ and $\hat{\mathbf{s}}_e$ as follows:

$$\hat{\mathbf{s}}_o = (\mathbf{K}_o)_{ell} / |\mathbf{K}_o| = (s_{oa}, s_{ob}, s_{oc})^T, \quad (38)$$

$$\hat{\mathbf{s}}_e = (\mathbf{K}_e)_{ell} / |\mathbf{K}_e| = (s_{ea}, s_{eb}, s_{ec})^T. \quad (39)$$

Yeh [5, chapter 9.2] has shown that the electric-field-vector directions are given by

$$(\hat{\mathbf{o}})_{ell} = (s_{ob}, -s_{oa}, 0)^T, \quad (40)$$

$$(\hat{\mathbf{e}})_{ell} = \left(\frac{s_{ea}}{n_e^2(\chi_e) - n_o^2}, \frac{s_{eb}}{n_e^2(\chi_e) - n_o^2}, \frac{s_{ec}}{n_e^2(\chi_e) - n_e^2} \right)^T, \quad (41)$$

where the refraction angle χ_e is given by equation 13 and $n_e(\chi_e)$ by equation 14. Substituting equations 38 and 39 into equations 40 and 41 we find

$$(\hat{\mathbf{o}})_{ell} = N_o(-\beta \cos \phi, \beta \sin \theta \sin \phi - K_{oz} \cos \theta, 0)^T, \quad (42)$$

$$(\hat{\mathbf{e}})_{ell} = N_e \left(\frac{K_{ez} \cos \theta - \beta \sin \theta \sin \phi}{n_e^2(\chi_e) - n_o^2}, \frac{-\beta \cos \phi}{n_e^2(\chi_e) - n_o^2}, \frac{K_{ez} \sin \theta + \beta \cos \theta \sin \phi}{n_e^2(\chi_e) - n_e^2} \right)^T, \quad (43)$$

where N_o and N_e are normalising constants. In the xyz frame of reference the vectors $\hat{\mathbf{o}}$ and $\hat{\mathbf{e}}$ are therefore given by

$$\hat{\mathbf{o}} = \mathcal{M}(\hat{\mathbf{o}})_{ell}, \quad (44)$$

$$\hat{\mathbf{e}} = \mathcal{M}(\hat{\mathbf{e}})_{ell}. \quad (45)$$

10 Tables

Wavelength of light (sodium D-line), λ	589.3nm
LC extraordinary refractive index, n_e	1.69
LC ordinary refractive index, n_o	1.50
Nylon alignment-layer refractive index, n_{nyl}	1.53
Glass refractive index, n_{gl}	1.54

Table 1: Optical constants used in the conoscopic calculations

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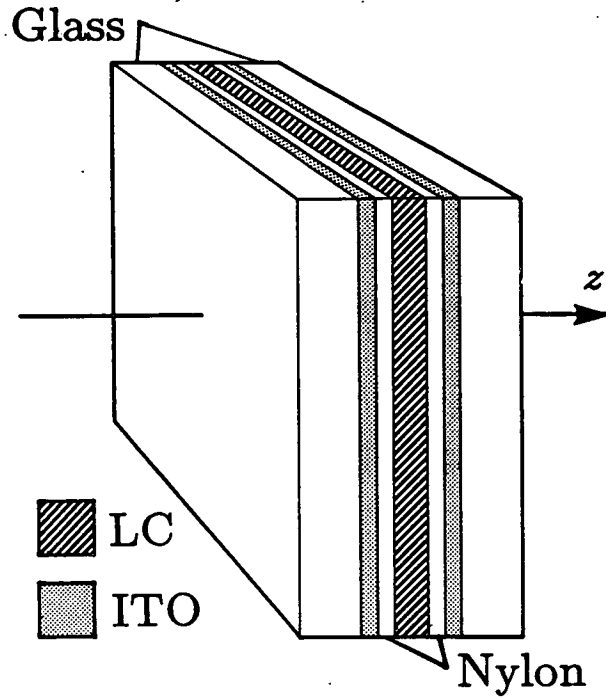


Figure 2 Schematic diagram of a LC cell showing the rubbed-nylon alignment layers, transparent indium tin oxide (ITO) electrodes and glass substrates. The z -axis is parallel to the principal optic axis of the microscope.

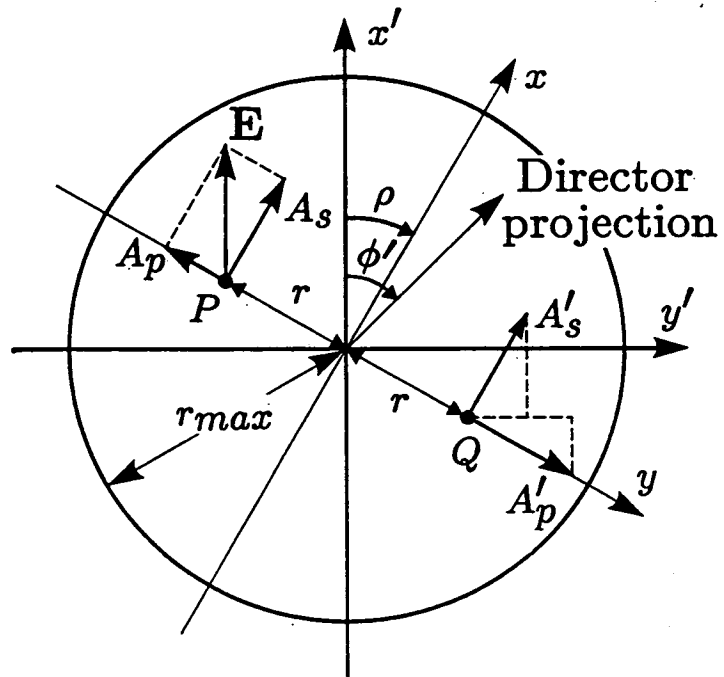


Figure 3 Coordinate system used in the conoscopic calculations. The x' and y' axes are parallel to the polariser and analyser axes respectively. Linearly polarised light is incident on the LC cell in the yz -plane (the z -axis points out of the page) with electric field components A_p and A_s parallel and perpendicular to the plane of incidence. Only the components of the output electric field vectors A'_p and A'_s parallel to the y' axis are transmitted by the analyser. P and Q are the conjugate points in the input and output planes.

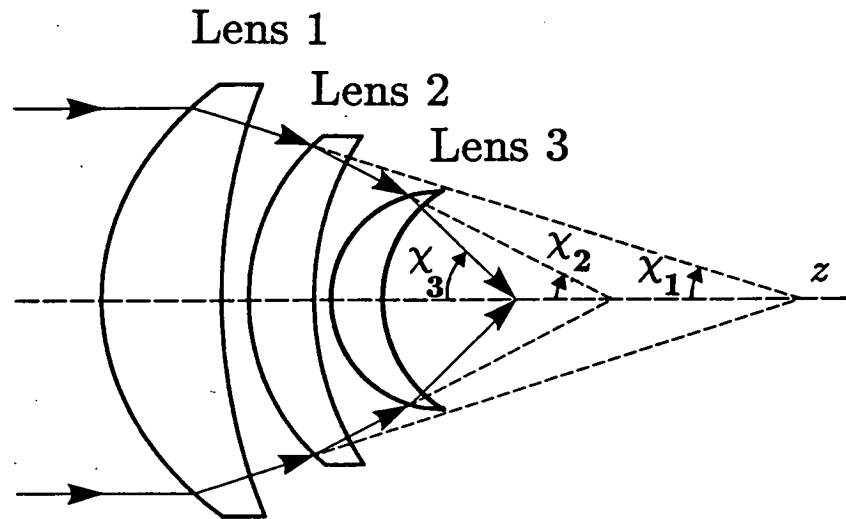


Figure 4 Lens triplet, consisting of a sphero-ellipsoidal (1) and two aplanatic (2 and 3) lenses, used to model the microscope condenser lens system. The same triplet was reversed to model the objective lens system.

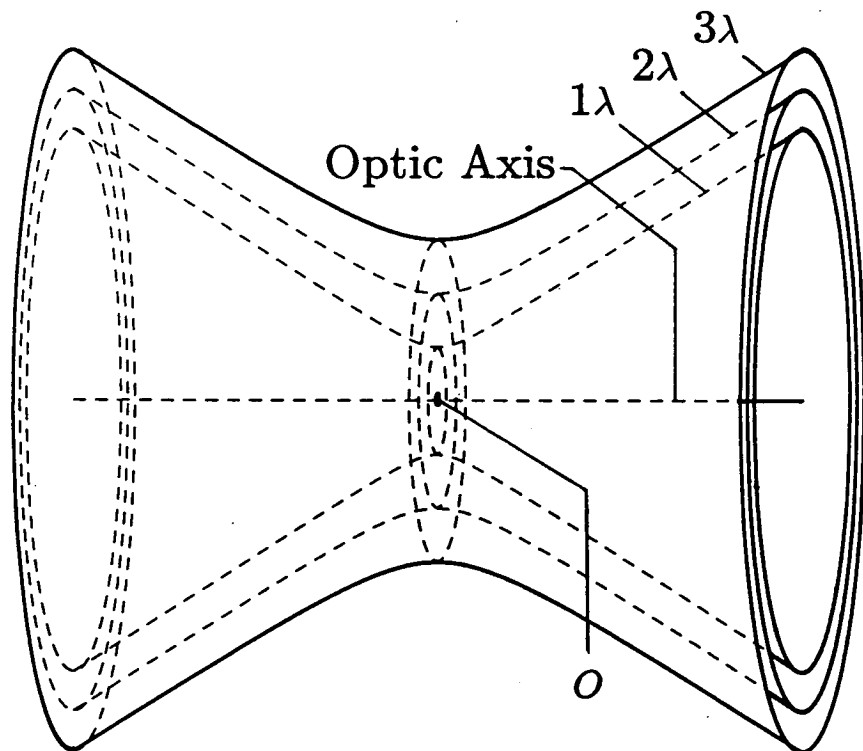


Figure 5 Centre sections of the first three Bertin's surfaces corresponding to phase differences of one, two and three wavelengths. The surfaces connect points of equal phase-difference between ordinary and extraordinary waves emanating from the point O .

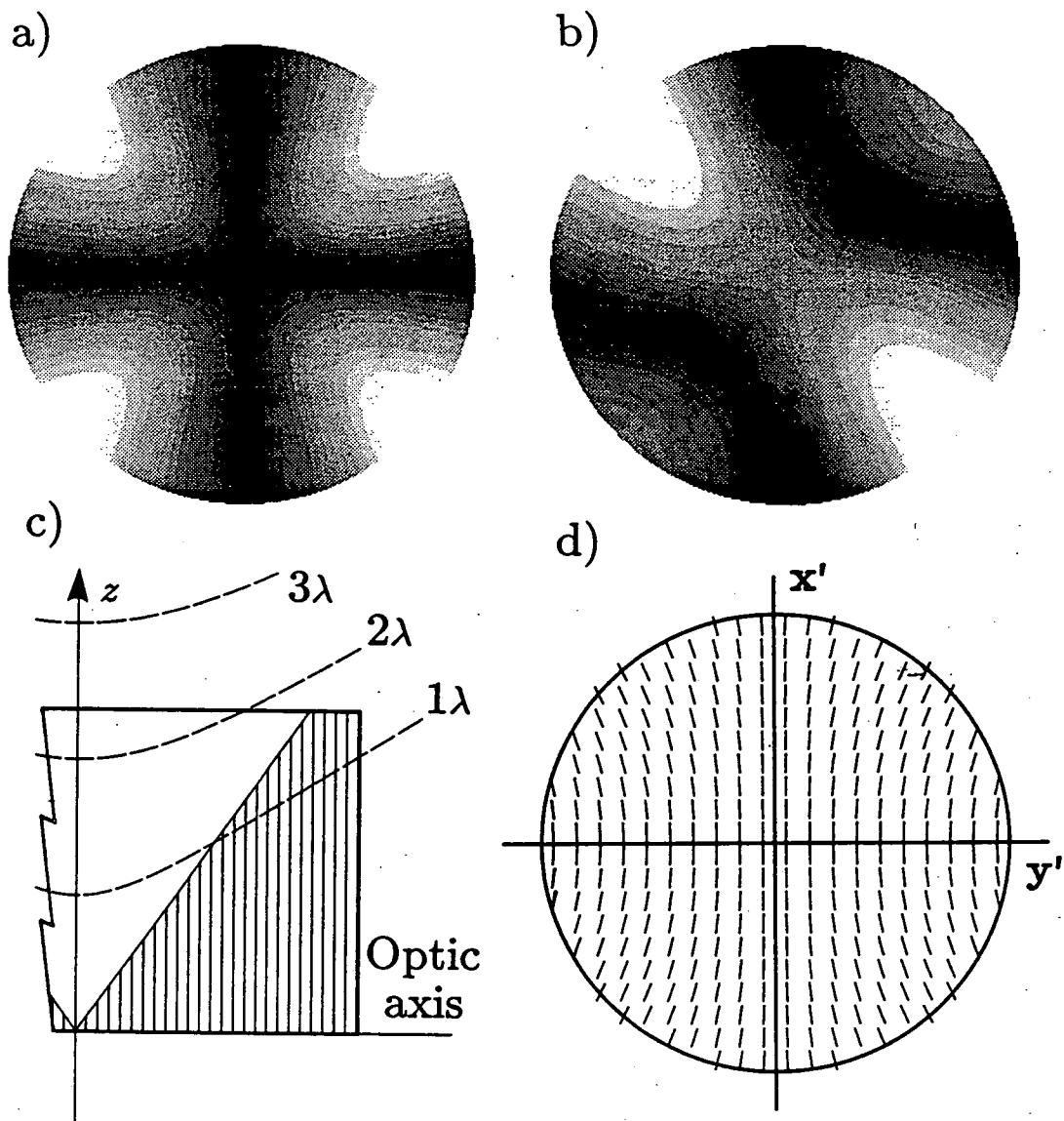


Figure 6 The “symmetric flash figure” produced by a cell containing homogeneously aligned LC with no director tilt ($\theta = 0$) and a) $\phi' = 0$ and b) $\phi' = 3^\circ$. In a) the isogyres form a dark cross which breaks up into two hyperbolic isogyres as shown in b) when the sample is rotated.

c) A cross-section of the LC layer showing the cone of light and the Bertin's surfaces. The intersection of the 2λ -surface with the LC surface, the 2λ -isochrome, causes the broadening of the vertical arms of the isogyres relative to the horizontal arms but no other part of the isochrome is visible.

d) Rotation of the polarisation of light by Fresnel refraction at the surfaces of an isotropic slab on the microscope stage. The polarisation rotation (away from the x' -axis) has been exaggerated by a factor of four and was calculated for a slab with a refractive index of 1.6. It is this effect which obscures the isochrome in a) and b).

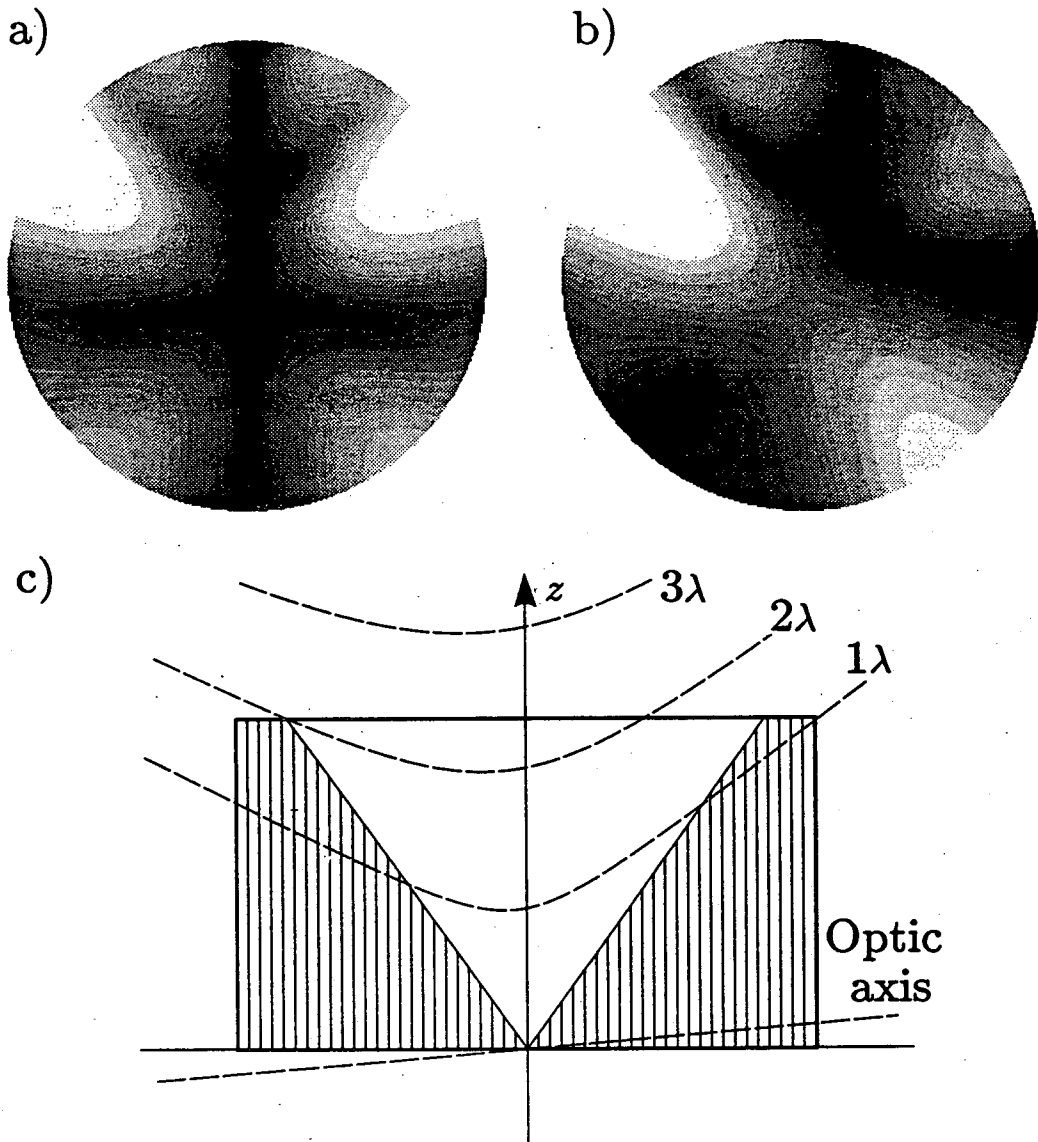


Figure 7 Conoscopic figures produced by a LC cell with $\theta = 5^\circ$ and a) $\phi' = 0$ and b) $\phi' = 3^\circ$. The 2λ Bertin's surface shown in c) produces the isochrome in the top part of the figures. When the LC cell is rotated the isogyre breaks in two but the isochrome rotates unchanged with the cell.

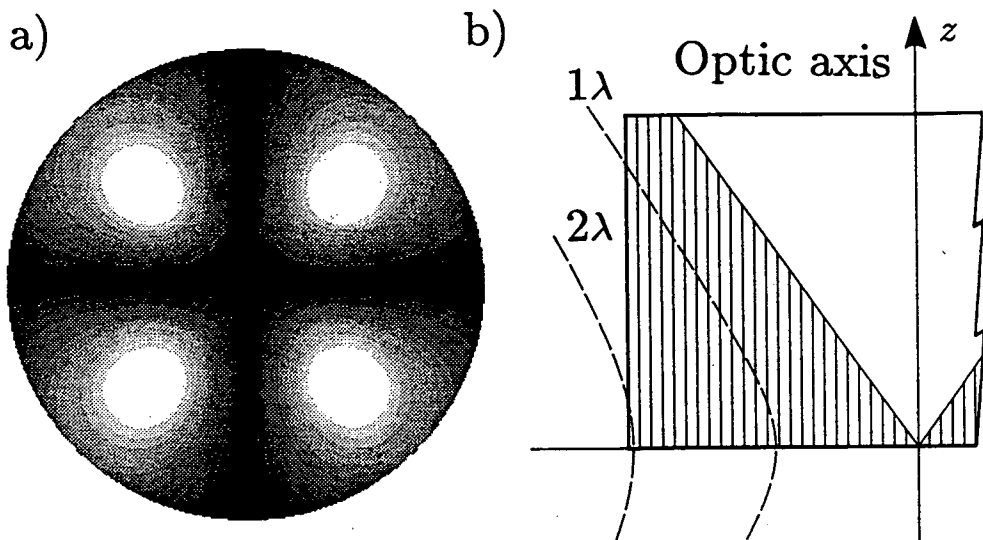


Figure 8 a) The optic-normal ($\theta = 90^\circ$) conoscopic figure and b) the corresponding orientation of Bertin's surfaces. No isochromes are visible as none of the Bertin's surfaces intersect the LC surface within the field of view.

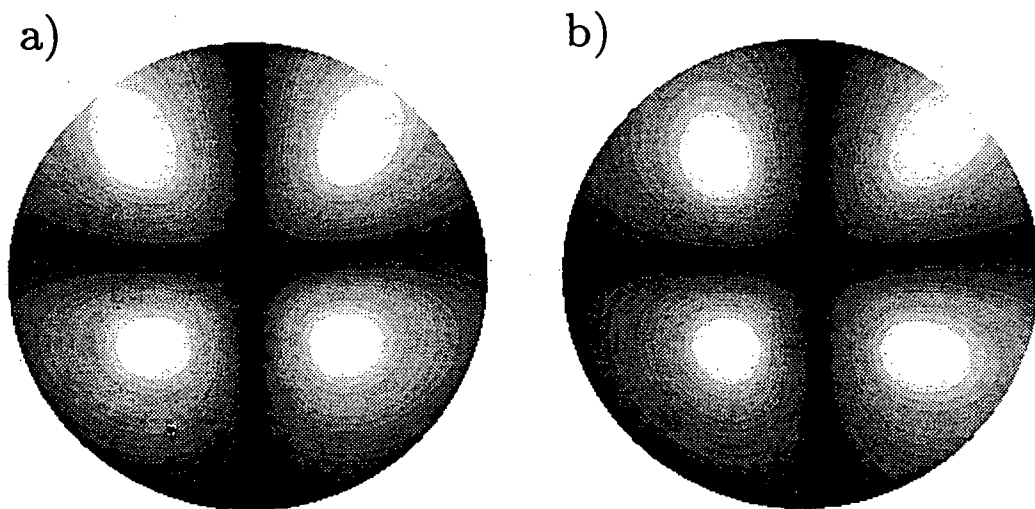


Figure 9 Conoscopic figures produced by a LC cell with $\theta = 85^\circ$ and a) $\phi' = 0$ and b) $\phi' = 45^\circ$. The centre of the isogyre cross lies directly over the LC optic axis in both figures and the cross retains its orientation as the LC cell is rotated.

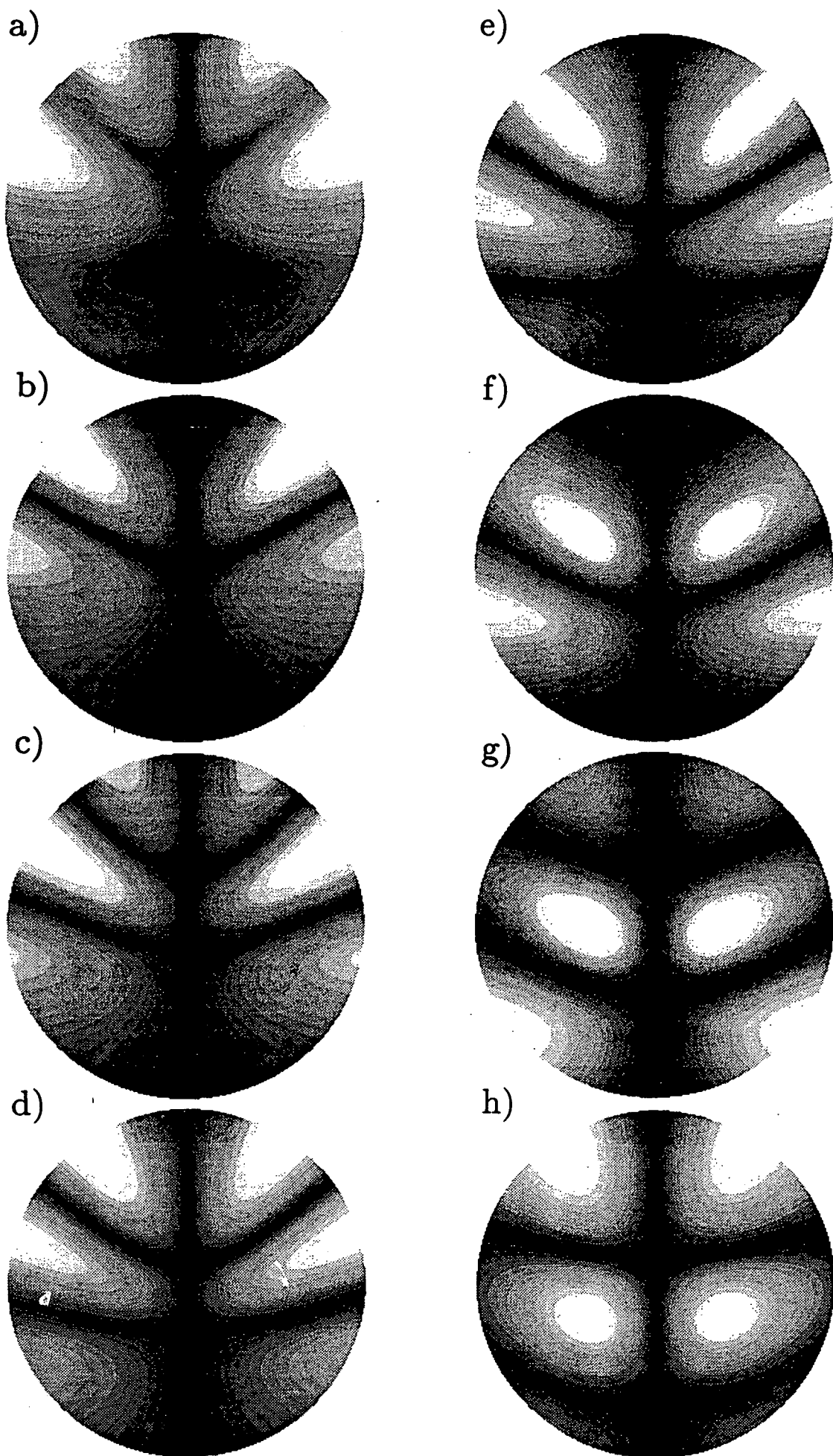


Figure 10 Conoscopic figures produced by a LC cell with a) $\theta = 10^\circ$, b) $\theta = 20^\circ$, c) $\theta = 30^\circ$, d) $\theta = 40^\circ$, e) $\theta = 50^\circ$, f) $\theta = 60^\circ$, g) $\theta = 70^\circ$ and h) $\theta = 80^\circ$. As the tilt angle increases the 1λ -isochrome and then the optic axis enter the field-of-view and finally the 2λ -isochrome leaves the field-of-view.

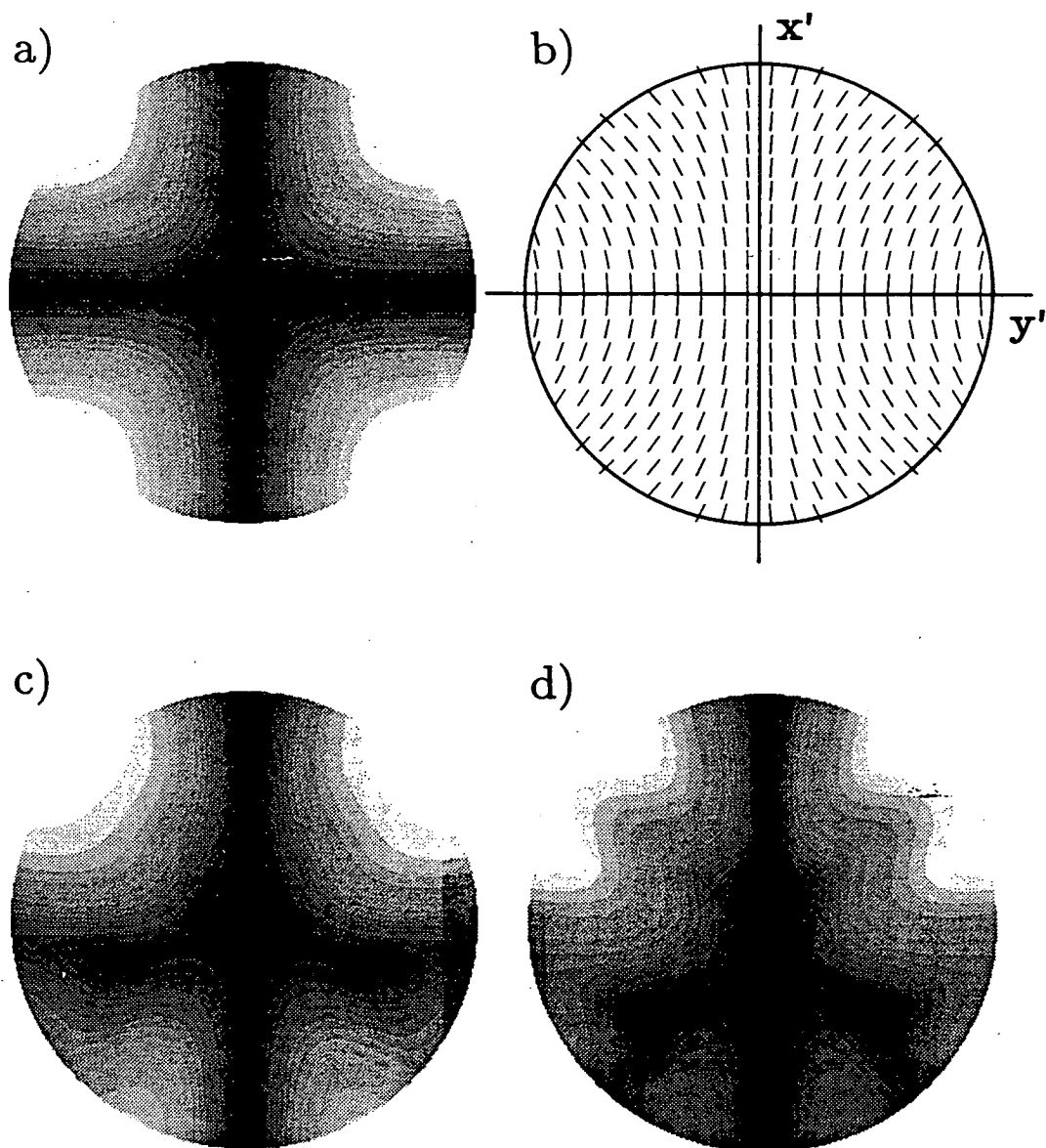
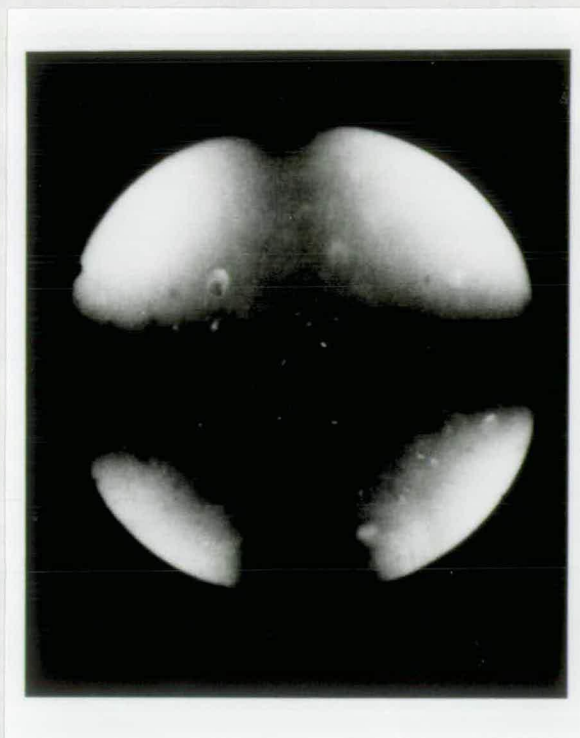
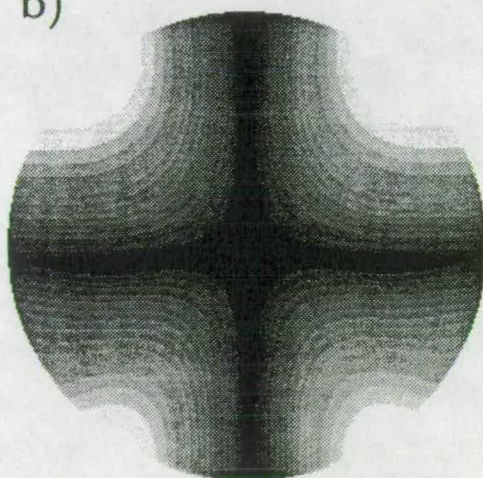


Figure 11 a) The “isotropic cross” produced by a pair of the triplet lens shown in figure 4 when the LC cell is removed. This figure is a result of the lens-induced polarisation rotation shown (exaggerated by a factor of four) in b). When the lens-induced polarisation is taken into account the conoscopic figures are altered as shown in c) for $\theta = 5^\circ$ (cf figure 7a) and d) for $\theta = 10^\circ$ (cf figure 10a).

a)



b)



c)

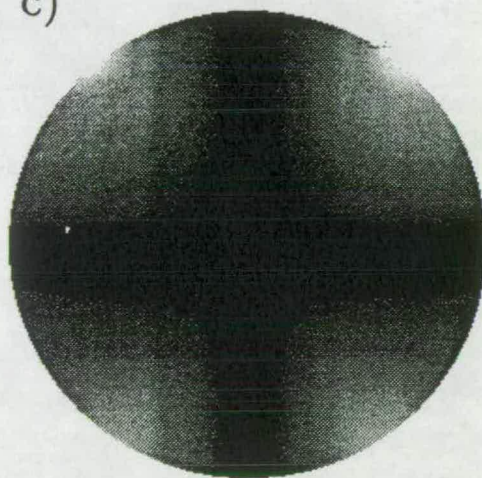


Figure 12 a) Conoscopic figure produced by a $7\mu\text{m}$ thick layer of chiral smectic C liquid crystal. This was compared with calculated conoscopic figures with tilt angles (θ) of 0 to 5° in 1° steps. The closest match was with the $\theta = 2^\circ$ figure shown in b) image-processed and c) as calculated.

A Method for Computing the Optical Properties of a Smectic C* Liquid Crystal Cell with a Chevron Layer Structure

Alastair R. MacGregor

August 22, 1989

Abstract

In this paper a model developed previously[†] for computing the director orientation in a cell containing chiral smectic C liquid crystal (SmC* LC) is extended to include a chevron layer structure in the relaxed (zero voltage) state. Results of the director orientation calculations are presented and used in a formalism developed elsewhere[‡] to compute the transmittance of a $7\mu\text{m}$ thick cell for different azimuthal orientations of the cell between crossed polarisers. It is shown that the theoretical and measured orientations which give minimum transmittance are in good agreement over the entire voltage range considered (0–20V). The computed average director tilt angle is found to be consistent with conoscopic measurements performed with a polarising microscope. Finally, on the basis of the computed director orientations, an explanation is given of why the zero-voltage minimum transmission orientation angle is so much smaller in thick ($\sim 7\mu\text{m}$) SmC* LC cells than it is in thin ($\sim 2\mu\text{m}$) cells.

†A. R. MacGregor, "A Method for Computing the Optical Properties of a Smectic C* Liquid Crystal Cell", J. Opt. Soc. Am. A **6**, September 1989.

‡D. W. Berreman, "Optics in Smoothly Varying Anisotropic Planar Structures: Application to Liquid Crystal Twist Cells", J. Opt. Soc. Am. **63**, 1374–1380 (1973).

Equations 17 to 19 are solved by discretising the space and time coordinates into steps of length Δx and Δt respectively and using the fourth order Runge–Kutta method as described in reference [6]. Since the chiral elastic constants have been set to zero the values of ϕ and ψ are antisymmetric about the chevron interface and it is only necessary to solve equations 17 to 19 for ϕ and ψ over the range $x \in [0, d/2]$. In the range $x \in [d/2, d]$, ϕ and ψ are given by the relationships

$$\phi(d - x_o) = -\phi(x_o), \quad (21)$$

$$\psi(d - x_o) = -\psi(x_o). \quad (22)$$

The starting configuration for ϕ in the range $x \in [0, d/2]$ is taken to be a linear variation from $\phi = -90^\circ$ at $x = 0$ to $\phi = -55.8^\circ$ (the value computed by setting $\beta = 0$ and solving equation 6 for ϕ) at $x = d/2$ and for ψ is taken to be a constant value of -21.5° . The antisymmetry of ϕ and ψ also makes the x -component of $\mathbf{P}_s$ symmetric about the chevron interface so that E_x is symmetric. If a voltage V is applied across the LC then

$$\Phi(d - x_o) = V - \Phi(x_o) \quad (23)$$

and in particular $\Phi(d/2) = V/2$. Therefore equation 20 need only be solved over the range $x \in [0, d/2]$ subject to the boundary conditions that $\Phi(0) = 0$ and $\Phi(d/2) = V/2$. For a given set of ϕ and ψ values equation 20 can be solved efficiently in the following way. First the equation is written in its finite difference form:

$$\epsilon_o \epsilon_\perp \left[\frac{\Phi_{i+1} - 2\Phi_i + \Phi_{i-1}}{(\Delta x)^2} \right] = P_s \left[\left(\frac{\psi_{i+1} - \psi_{i-1}}{2\Delta x} \right) \sin \psi_i \cos \phi_i + \left(\frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} \right) \cos \psi_i \sin \phi_i \right] \quad (24)$$

where each subscript refers to the x -coordinate of the variable i.e. Φ_{i+1} is the value of Φ at $x = (i+1)\Delta x$. i runs from 0 at $x = 0$ to N at $x = d$. A finite difference equation in the form of equation 24 can be written down for each point along the x -axis between $x = 0$ and $x = d/2$ (not including the end points where the potential is already known). These equations are then written in the form of a tridiagonal matrix equation:

$$\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \vdots \\ \Phi_{N/2-2} \\ \Phi_{N/2-1} \end{pmatrix} = \begin{pmatrix} D_1 - \Phi_0 \\ D_2 \\ D_3 \\ \vdots \\ D_{N/2-2} \\ D_{N/2-1} - \Phi_{N/2} \end{pmatrix} \quad (25)$$

where D_i is the right hand side of equation 24 multiplied by $(\Delta x)^2/\epsilon_o \epsilon_\perp$, $\Phi_0 = 0$ and $\Phi_{N/2} = V/2$. Finally equation 25 is solved for the vector $(\Phi_1, \Phi_2, \dots, \Phi_{N/2-1})^T$ using a library band-matrix solver (for example the NAG library routines F01LEF and F04LEF).

Table 1 lists the physical properties of the B.D.H. LC SCE3 which were used in the calculation of the director orientation.

Once a set of values of ϕ and ψ is known the method of calculating the optical transmittance developed by Berreman [19] and Montgomery [20,21] is applied to the

5 Appendix: Coefficients of the Minimum Free Energy Equation

The forms of the Γ_i in equations 17 and 19 are:

$$\begin{aligned}
 \Gamma_1 &= -\cos^2 \psi (B_1 \sin^2 \phi + B_2 \cos^2 \phi) - B_3 \sin^2 \psi, \\
 \Gamma_2 &= B_2 \cos \psi \cos \phi \sin \psi \sin \phi, \\
 \Gamma_3 &= -\frac{1}{2}(B_1 - B_2) \cos^2 \psi \sin 2\phi, \\
 \Gamma_4 &= \cos^2 \psi \cos \phi \sin \phi (B_2 - A \cos 2\phi), \\
 \Gamma_5 &= \sin 2\psi (B_1 \sin^2 \phi + B_2 \cos^2 \phi - B_3), \\
 \Gamma_7 &= -P_e E \cos \psi \sin \phi, \\
 \Gamma_8 &= \Gamma_1, \\
 \Gamma_9 &= \Gamma_2, \\
 \Gamma_{11} &= -2\sigma_{nem} \sin \beta \cos \psi \cos \phi \sin \theta - \\
 &\quad 2\sigma_{al} \sin \alpha \left(\frac{\sin \phi \sin \theta}{\cos \beta} + \frac{\cos^2 \phi \sin^2 \theta \cos \psi \sin \beta}{\cos^3 \beta} \right).
 \end{aligned}$$

The forms of the Λ_i in equation 18 are:

$$\begin{aligned}
 \Lambda_1 &= -B_2 \sin^2 \psi \sin^2 \phi - A \cos^2 \psi (1 - \sin^2 \phi \cos^2 \phi), \\
 \Lambda_2 &= B_2 \cos \psi \cos \phi \sin \psi \sin \phi, \\
 \Lambda_3 &= \frac{1}{2} \sin 2\psi [B_3 - \sin^2 \phi (B_1 + B_2)], \\
 \Lambda_4 &= \frac{1}{2} A \sin 2\psi (1 - \sin^2 \phi \cos^2 \phi) - \frac{1}{2} B_2 \sin 2\psi \sin^2 \phi, \\
 \Lambda_5 &= \frac{1}{2} A \cos^2 \psi \sin 4\phi - B_2 \sin^2 \psi \sin 2\phi, \\
 \Lambda_7 &= -P_e E \sin \psi \cos \phi.
 \end{aligned}$$

6 Acknowledgements

I am indebted to Mr R.M.Sillitto, Dr D.G.Vass, Dr R.C.Dougal and other members of the Applied Optics group of the Department of Physics for helpful discussions. Dr W.A.Crossland and Mr M.F.Bone (S.T.C. Technology Ltd.) have given both stimulus and encouragement and their company generously provided the LC cells used. Finally the award of an S.E.R.C. C.A.S.E. award with S.T.C. Technology Ltd. is gratefully acknowledged.

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7 Tables

Spontaneous polarisation, P_s	$88\mu C m^{-2}$
Cone angle, θ	25.5°
Parallel dielectric constant, $\epsilon_{ }$	3.10
Perpendicular dielectric constant, $\epsilon_{\perp}$	5.04

Table 1: Specification of the B.D.H. LC SCE3 at $15^\circ C$

Material	Thickness
Liquid crystal (B.D.H. SCE3)	$7\ \mu m$
Nylon	$0.1\ \mu m$
ITO	$0.05\ \mu m$
Glass	1 mm

Table 2: Specification of the LC cell

LC extraordinary refractive index, n_e	1.69
LC ordinary refractive index, n_o	1.50
Nylon refractive index, n_{nyl}	1.53
ITO refractive index, n_{ITO}	2.0
Glass refractive index, n_{gl}	1.54

Table 3: Optical constants used in the calculation

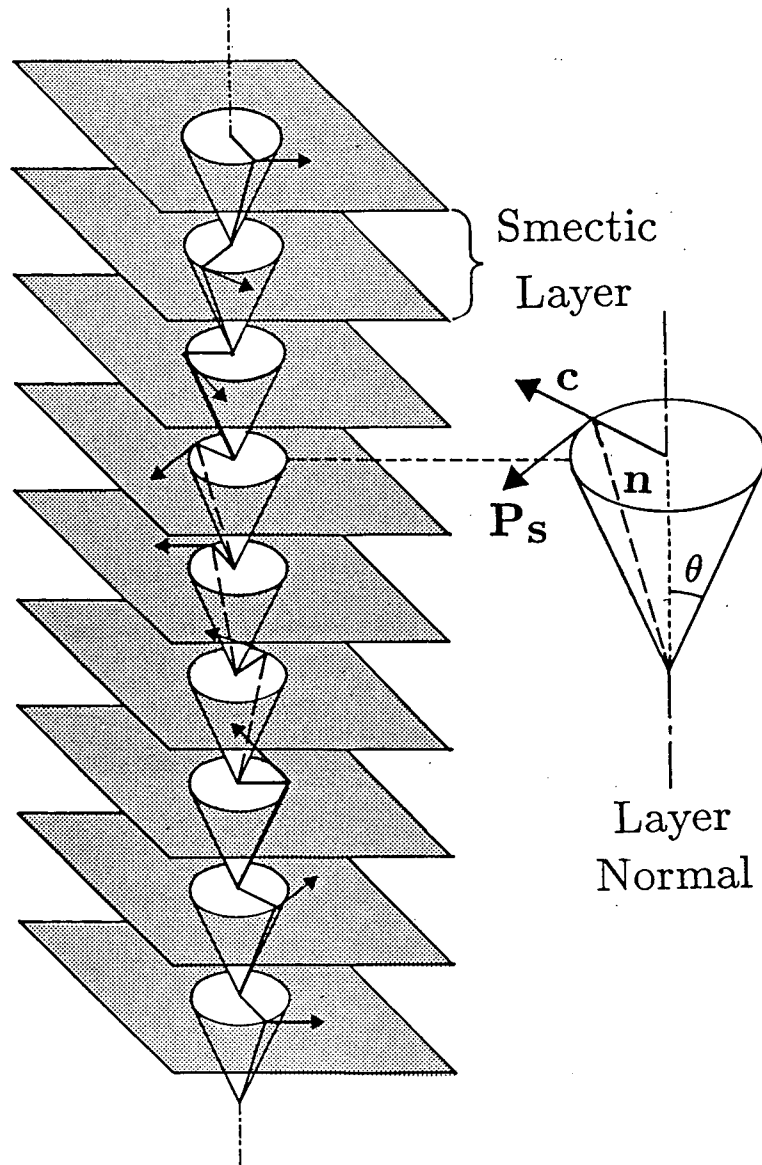


Figure 1: Director configuration in a bulk sample of SmC* LC. Within each smectic layer the $\mathbf{n}$ -director makes a constant angle θ with the layer normal and precesses about the layer normal from layer to layer. The spontaneous polarisation $\mathbf{P}_s$ lies in the smectic layer plane and perpendicular to the projection of the $\mathbf{n}$ -director onto the plane. This projected direction also defines the $\mathbf{c}$ -director orientation.

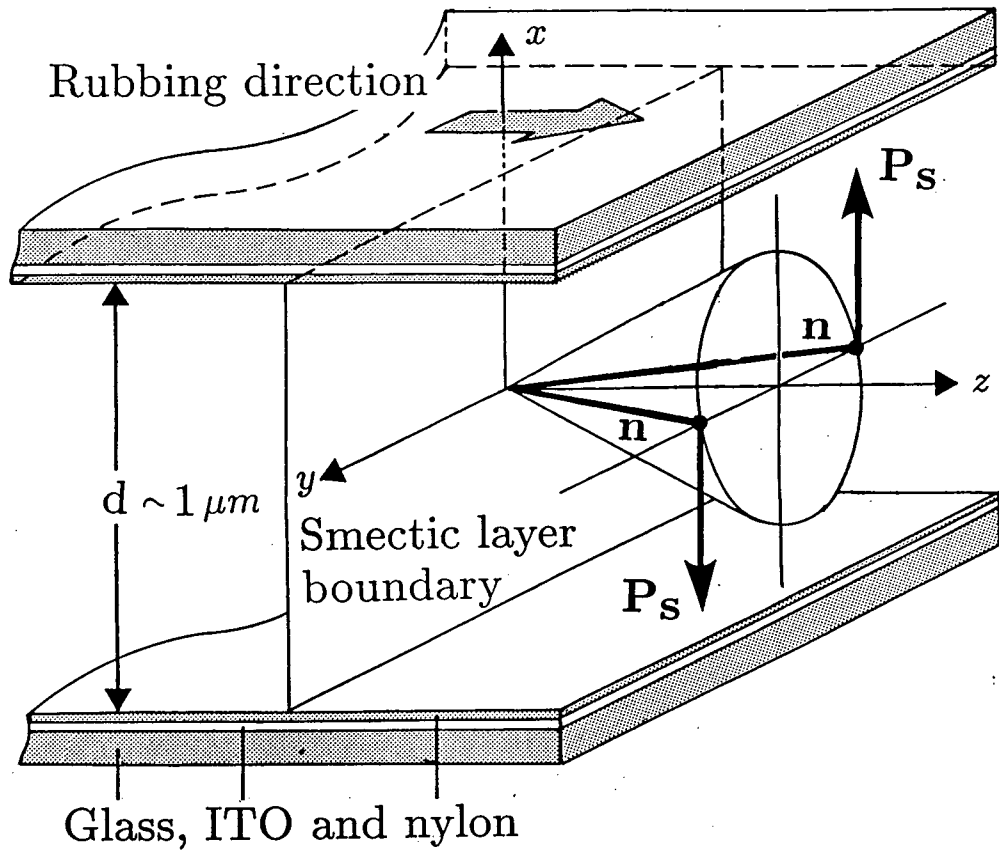


Figure 2: Ideal SSFLC cell. Provided that the cell thickness is small compared with the pitch length of the helix shown in figure 1 the helix is prevented from forming by surface forces. The n -director takes up one of the two stable orientations shown symmetrically positioned on either side of the rubbing direction. If a d.c. voltage is applied across the cell the n -director can be switched from one orientation to the other.

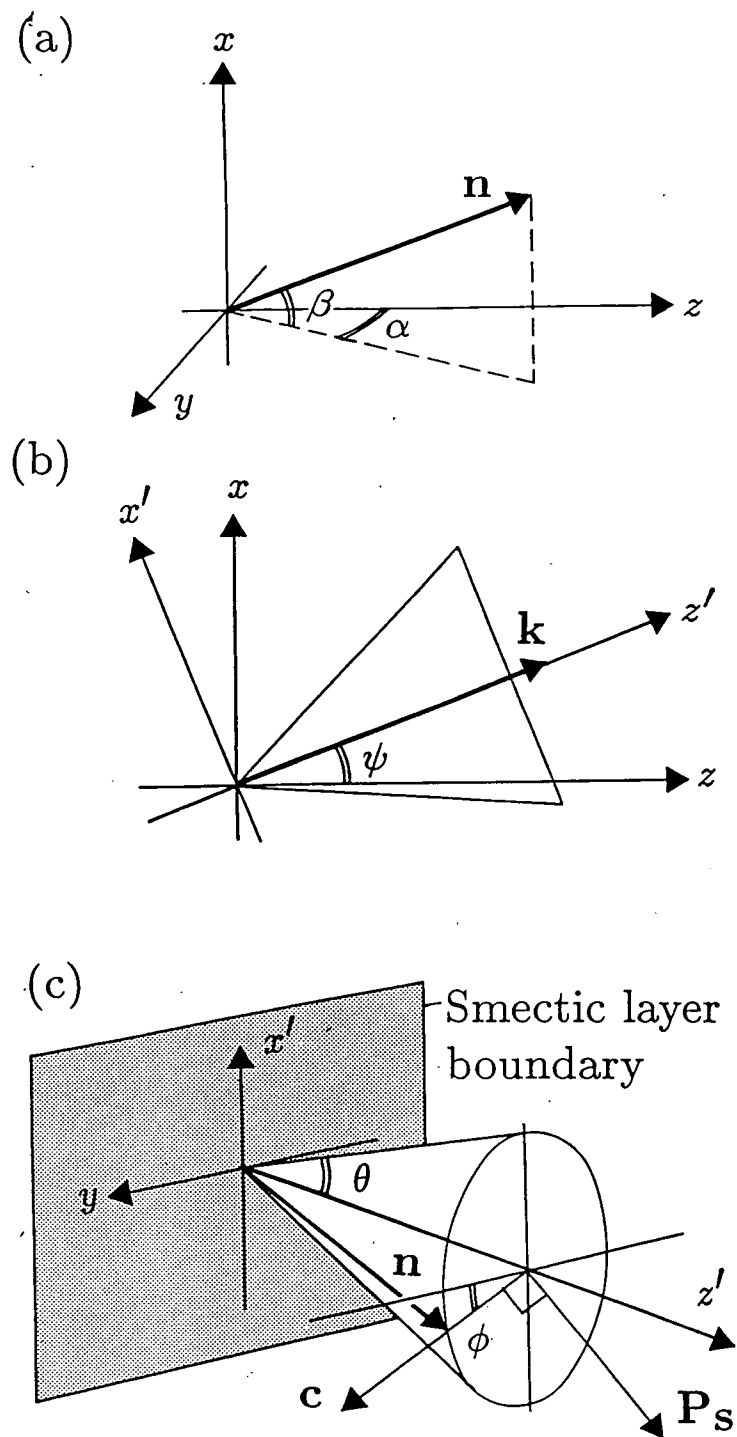


Figure 3: Coordinate system used in the theoretical formulation to describe the director orientation.

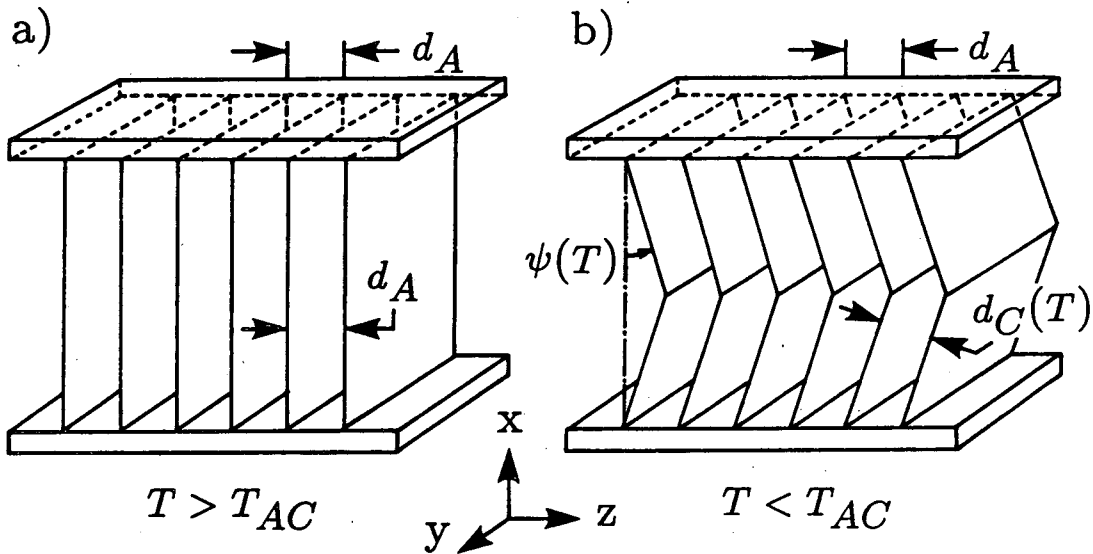


Figure 4: Schematic diagram of the smectic layer configuration in a) the *SmA* phase and b) the *SmC** phase. Above the *SmA*–*SmC** phase transition temperature, T_{AC} , the smectic layers are perpendicular to the LC surfaces. For temperatures below T_{AC} the smectic layers tilt at a temperature dependent angle, $\psi(T)$, away from the perpendicular. The smectic layer thickness in the *SmC** phase ($d_C(T)$) is related to the layer thickness in the *SmA* phase (d_A) and the layer tilt angle $\psi(T)$ by equation 7.

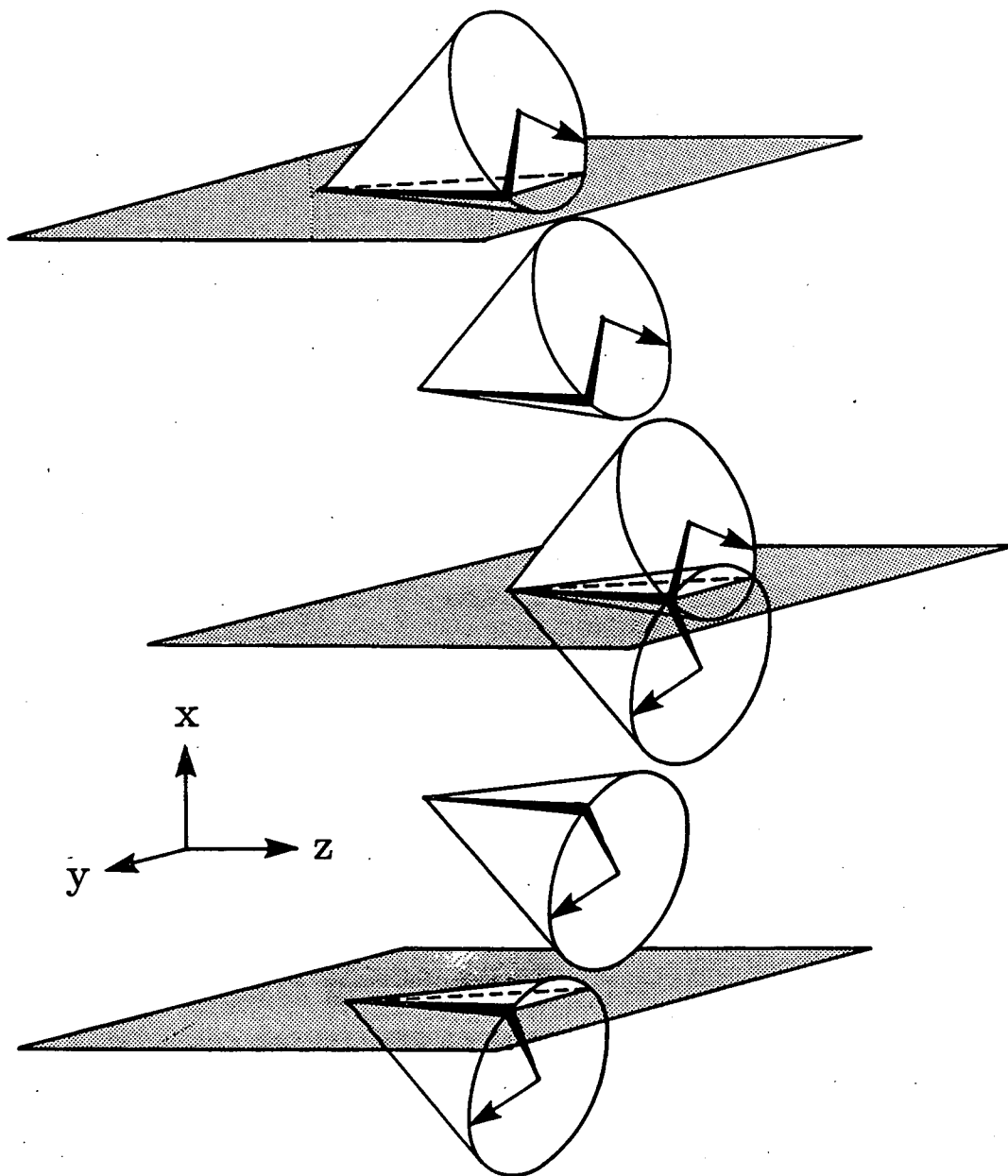


Figure 5: Schematic diagram of the uniform director configuration in a SmC* LC cell with a symmetric chevron layer structure. The cones represent the loci of possible director configurations, the lines on the conical surfaces represent the $\mathbf{n}$ -director orientations and the arrows on the cone bases represent the orientation of the spontaneous polarisation $\mathbf{P}_s$. At every point through the LC the $\mathbf{n}$ -director is parallel to the LC surfaces and the plane of the chevron interface.

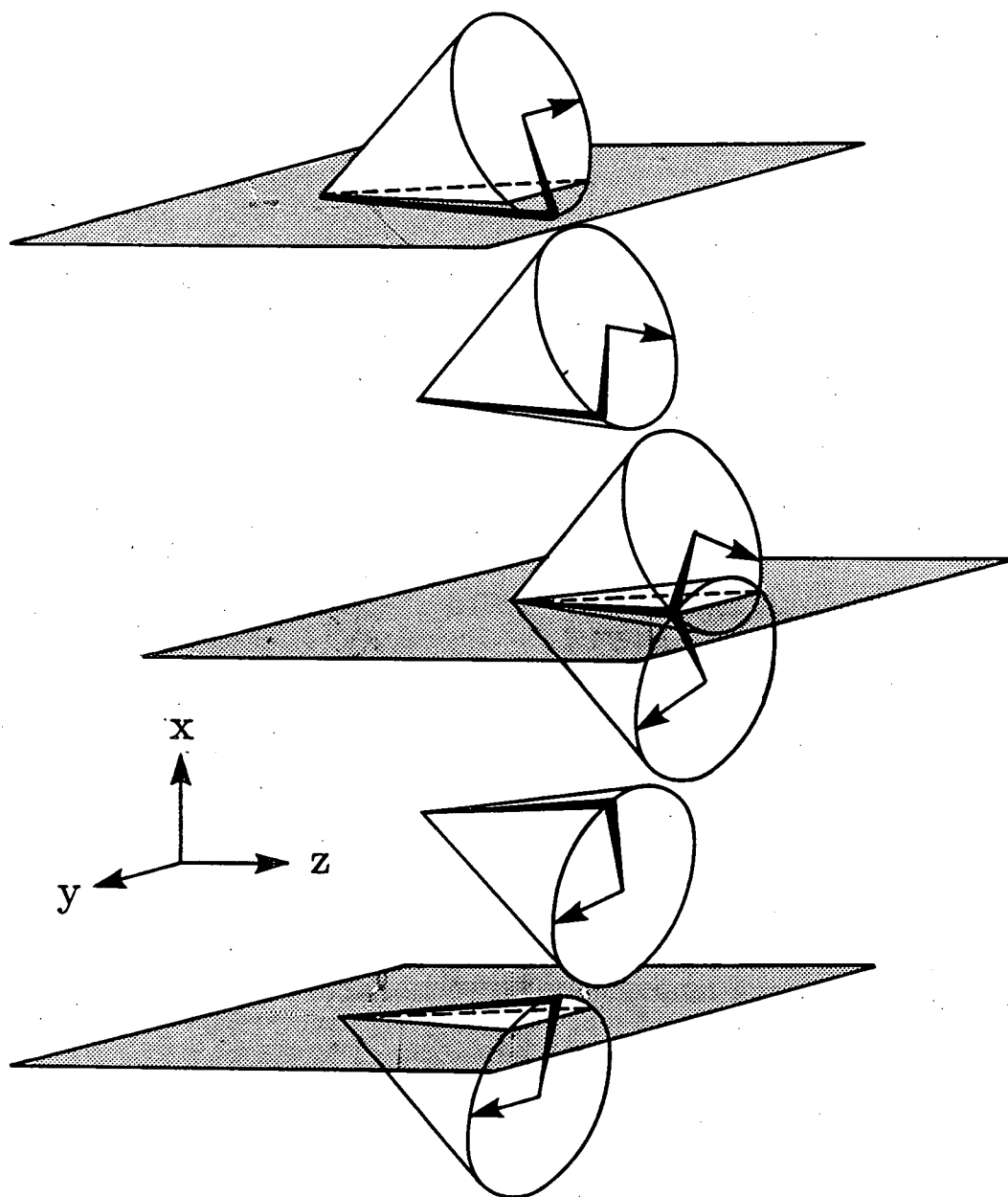


Figure 6: Director configuration proposed in this work. The layers are configured as a symmetric chevron in the relaxed (zero voltage) state and the director occupies one of the two positions defined by the intersections of the cones at the chevron interface. At the LC surfaces the alignment layer forces the n-director round until it is nearly parallel to the z-axis (rubbing direction).

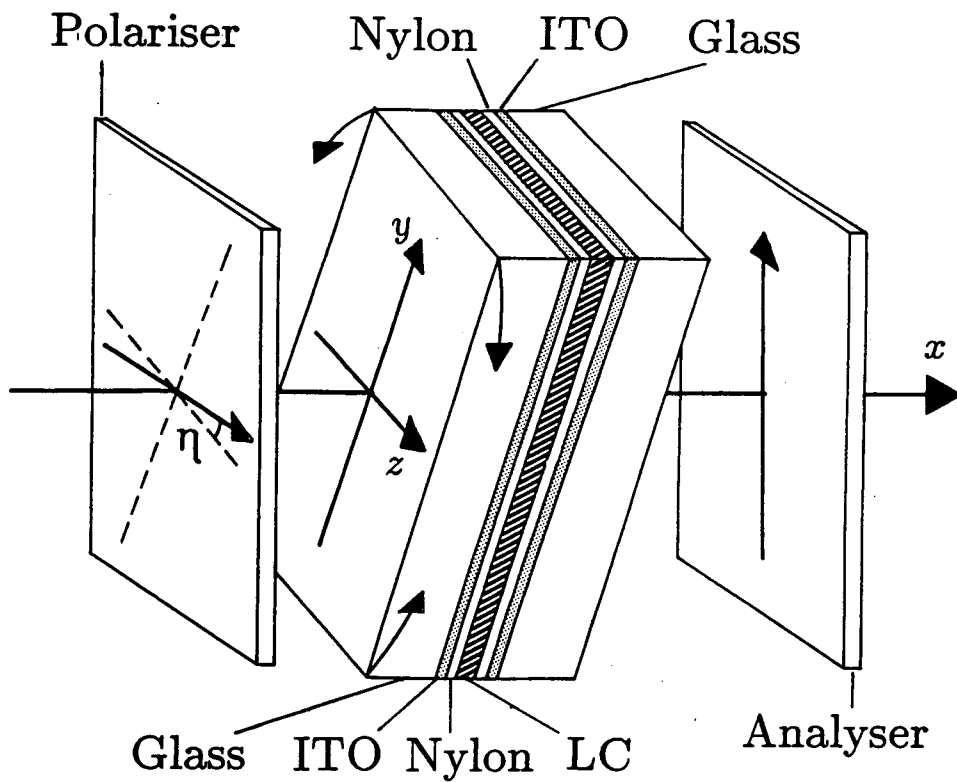


Figure 7: Model of the LC cell used in the optical calculations. The polariser and analyser are crossed and the LC cell is rotated about the x -axis to find the minimum transmission orientation. The rubbing direction is parallel to the z -axis and makes an angle η with the polariser axis.

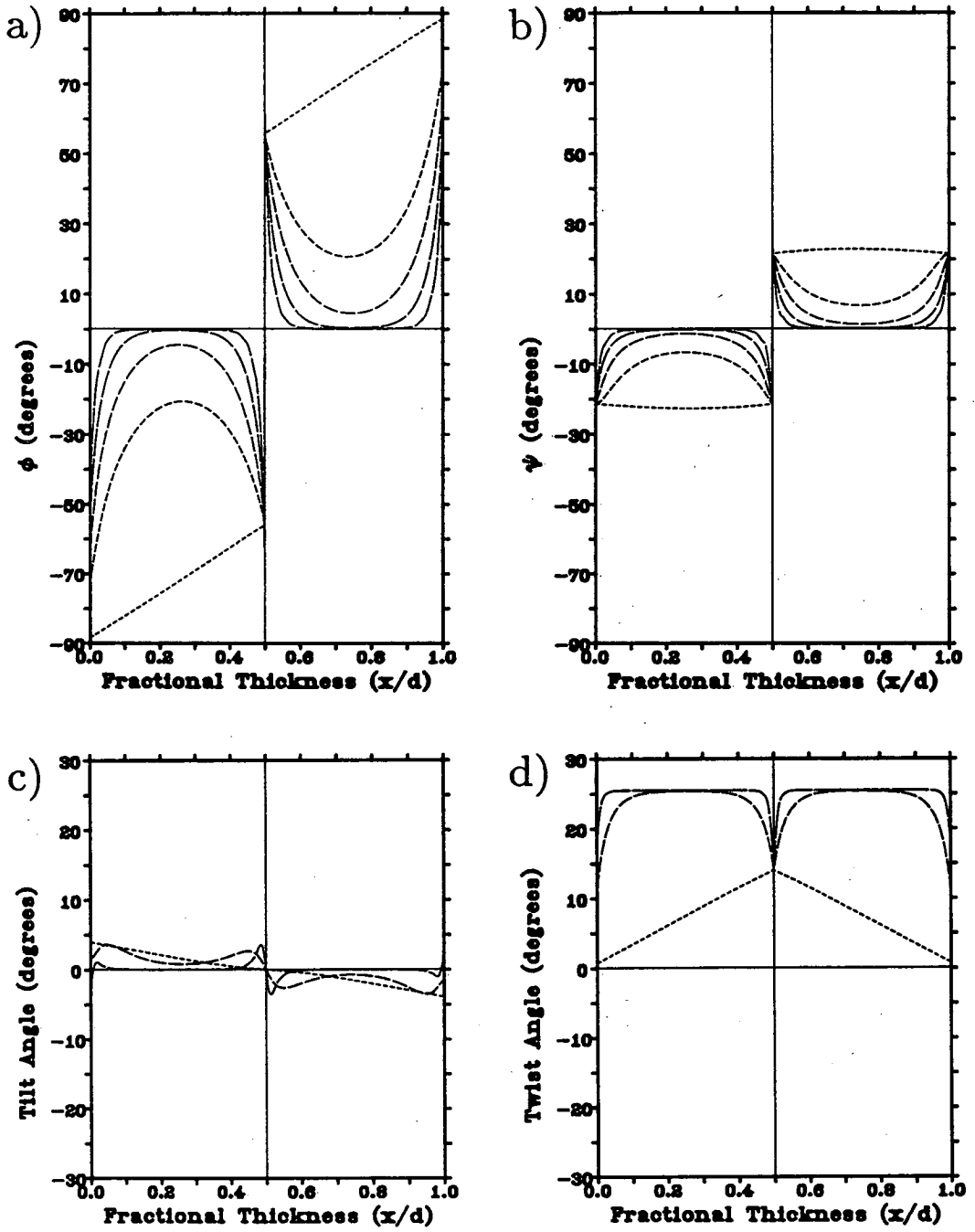


Figure 8: Computed variation of a) ϕ , b) ψ , c) tilt and d) twist with fractional distance through the $7\mu\text{m}$ thick LC cell. In a) and b) the curves are, in order of increasing dash length, for voltages of 0V, 0.25V, 1V, 4V and 16V. In c) and d) the curves are, in order of increasing dash length, for voltages of 0V, 1V and 16V.

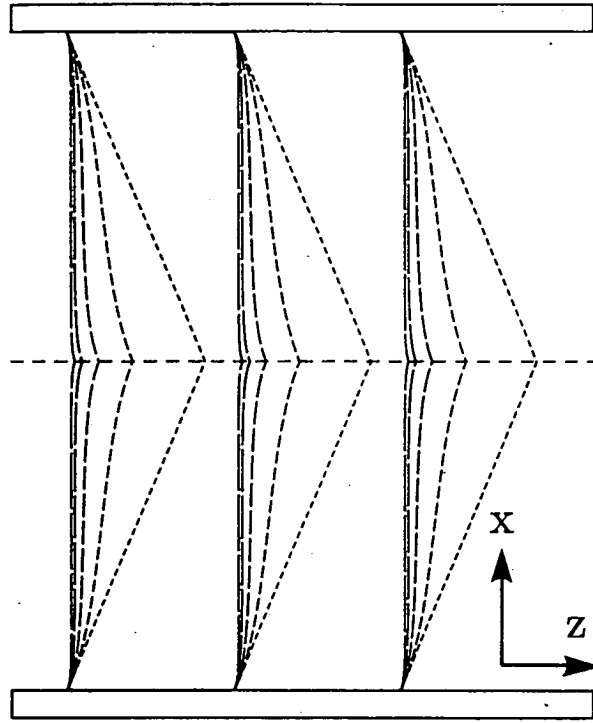


Figure 9: Calculated form of the smectic layers in a $7\mu\text{m}$ thick LC for various voltages. In order of increasing dash length the smectic layers are plotted for voltages of 0V, 0.25V, 1V, 4V and 16V.

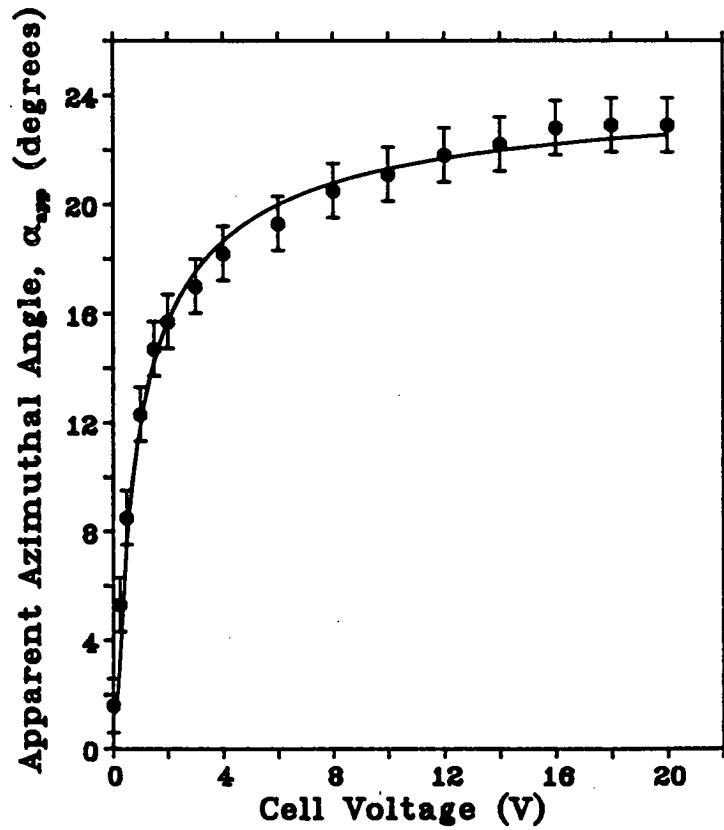


Figure 10: Variation of apparent azimuthal angle with LC cell voltage. The solid curve shows the computed points joined with a cubic spline and the points with the error bars represent the experimental measurements.