Invited Paper

Non-linear light propagation and bistability in nematic liquid crystals

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ABSTRACT

Liquid crystals can switch under influence of an electric field or under influence of incident light. In this paper we provide a mathematical description including electrical, optical and elastic torques. Depending on the applied voltage and the incident light, bistability in the director orientation may be possible. Under certain conditions, the sequence of applying incident TM polarized light and a static voltage allows to access different states.

Keywords: liquid crystals, nematics, reorientation, non-linearity, bistability, optical switching

1. INTRODUCTION

Anisotropic materials experience a torque in the presence of a static electric field, but also in the presence of electromagnetic radiation. The physical background of this effect is that the energy density in an anisotropic material can be reduced when the direction of highest polarizability aligns with the present electric field. In a liquid crystal, the director has the freedom to react to this 'optical' torque and the resulting reorientation leads to optical non-linearities. Such optical non-linearities have been studied extensively and the first observation of the reorientational nonlinearity was reported in 1980 [1]. The resulting nonlinearity is high compared to other material systems and even recently the high nonlinearity is studied in different configuration, e.g. with the z-scan technique [2,3]. The reorientational nonlinearity has also been used successfully to generate spatial optical solitons [4-6]. Optical bistability can also occur, for example in a Fabry-Perot cavity [7], but even without external feedback it is possible to induce bistability, for example by applying an externally applied magnetic field [8,9].

In this paper we investigate the reorientation of a one-dimensional liquid crystal layer under influence of the simultaneous presence of light and voltage. We develop a one-dimensional numerical model to determine the steady state director orientation profile and illustrate the model with numerical simulation results. Our model incorporates oblique angles of the incident light beam and we will demonstrate bistability by interplay between the optical field and applied voltage.

2. LC NON-LINEARITY FOR INCIDENT LIGHT

We consider a one-dimensional nematic liquid crystal layer between two electrode-covered substrates, without variation in the x and y direction. A TM polarized plane wave is entering from the bottom substrate (medium with refractive index n_m) making an angle θ_m with the z-axis. There is a voltage V_a applied over the electrodes on the top and bottom substrate. The liquid crystal director **L** is assumed to be lying in the xz-plane making an angle θ_L with the z-axis (inclination angle) and this angle is a function of the z-axis.

2.1 TM light propagation

For the optical modeling, we assume that the variations in the z-direction are small and that reflections can be neglected. In the liquid crystal the wave vector of the light makes an angle θ_k with the z-axis. The liquid crystal has ordinary and extra-ordinary refractive indices n_o and n_e and the effective refractive index for the given direction of the **k**-vector depends on the angle between **L** and **k**:

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Liquid Crystals XIII, edited by Iam Choon Khoo, Proc. of SPIE Vol. 7414
74140K · © 2009 SPIE · CCC code: 0277-786X/09/$18 · doi: 10.1117/12.827015

$$n_{\text{eff}} = \frac{n_e n_o}{\sqrt{n_e^2 \cos^2(\theta_L - \theta_k) + n_o^2 \sin^2(\theta_L - \theta_k)}} \tag{1}$$

In a one-dimensional structure, the periodicity in the x-direction should be the same as in medium m (the equality of the projection of the **k** vector on the xy plane), leading to the law of Snell:

$$n_{\text{eff}} \sin\theta_k = n_m \sin\theta_m \tag{2}$$

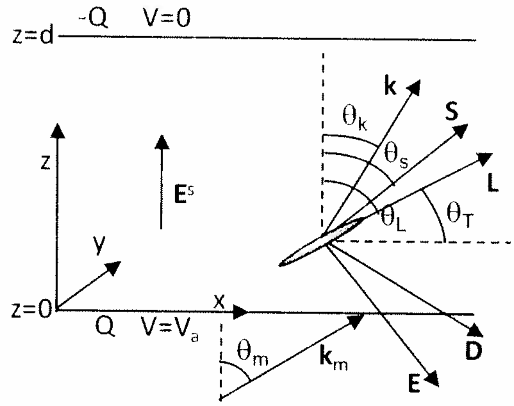

Fig. 1. Structure of the 1-dimensional LC device, indicating the applied voltage V_a, the charge Q on the electrodes, the static electric field, the incident light beam wave vector $\mathbf{k}_m$, the director **L** and the vectors **k**, **S**, **D**, **E** (with their respective inclination angles θ_k, θ_S, θ_D and θ_E) related to TM light in the liquid crystal (**D** is perpendicular to **k** and **E** is perpendicular to **S**). The tilt angle of the LC director is $\theta_T = 90^\circ - \theta_L$.

By combining both equations, the angle θ_k of the propagation vector in the liquid crystal can be found when θ_L and θ_m are given. The displacement field **D** is perpendicular to the **k**-vector, and because the material is anisotropic, the **E**-field usually makes an angle with the **D**-field. The **D** and **E**-field have a component along the liquid crystal director, which we call the extra-ordinary component D_e and E_e and a component perpendicular to **L** (in the xz-plane) which we call the ordinary component D_o and E_o. The ratio of the ordinary over the extra-ordinary component of the **D** (or **E**)-field is equal to the tangens of the angle between the **D** (or **E**)-field and director **L**. The ordinary (or extra-ordinary) components of the **D**-field and the **E**-field are related by the ordinary (or extra-ordinary) dielectric constant. Combining these relations gives:

$$\begin{aligned} \tan(\theta_D - \theta_L) &= \frac{D_o}{D_e} = \frac{\varepsilon_0 n_o^2 E_o}{\varepsilon_0 n_e^2 E_e} = \frac{n_o^2}{n_e^2} \tan(\theta_E - \theta_L) \\ \Rightarrow \tan(\theta_L - \theta_S) &= \frac{n_o^2}{n_e^2} \tan(\theta_L - \theta_k) \end{aligned} \tag{3}$$

The latter equation is based on the fact that **D** is perpendicular to **k** and **E** is perpendicular to **S**. This equation relates the direction of the vectors **L**, **k** and **S**. The field components refer to the amplitudes of the oscillating fields.

The magnitude of the D and E field are related by (again separating the ordinary and extra-ordinary components of the **D**-field):

$$D=\sqrt{\varepsilon_0^2 n_o^4 E^2 \sin^2(\theta_E-\theta_L)+\varepsilon_0^2 n_e^4 E^2 \cos^2(\theta_E-\theta_L)}$$
$$=\varepsilon_0 E\sqrt{n_o^4 \cos^2(\theta_L-\theta_S)+n_e^4 \sin^2(\theta_L-\theta_S)} \quad (4)$$
$$=\varepsilon_0 n_{\text{eff}}^2 E\cos(\theta_S-\theta_k)$$

The last equality is based on the relation between the angles θ_L, θ_S and θ_k. The magnetic field along the y direction can directly be determined from the magnitude of the D-field:

$$H_y=\frac{\omega}{k}D=\frac{c}{n_{\text{eff}}}D=\varepsilon_0 c n_{\text{eff}} E\cos(\theta_S-\theta_k) \quad (5)$$

The (time-averaged) Poynting vector **S** gives the direction and magnitude of the power flux associated with the light:

$$\mathbf{S}=\tfrac{1}{2}\mathbf{E}\times\mathbf{H}$$
$$S=\tfrac{1}{2}EH_y=\tfrac{1}{2}c\varepsilon_0 n_{eff} E^2\cos(\theta_S-\theta_k) \quad (6)$$

When partial reflections are neglected (the contrast in refractive indices is usually small), then the projection of the power on the z-direction should be independent of z (and equal to the value in the substrate medium m):

$$S_z=\tfrac{1}{2}c\varepsilon_0 n_{\text{eff}} E^2\cos(\theta_S-\theta_k)\cos\theta_S=\tfrac{1}{2}c\varepsilon_0 n_m E_m^2\cos\theta_m \quad (7)$$

The time-averaged torque that the light induces on the liquid crystal is given by:

$$\mathbf{\Gamma}^o=\tfrac{1}{2}\varepsilon_0\left(n_e^2-n_o^2\right)(\mathbf{L}\cdot\mathbf{E})(\mathbf{L}\times\mathbf{E})$$
$$\Gamma_y^o=\tfrac{1}{2}\varepsilon_0\left(n_e^2-n_o^2\right)\sin(\theta_L-\theta_S)\cos(\theta_L-\theta_S)E^2 \quad (8)$$

This torque is zero if the Poynting vector **S** is parallel or perpendicular to the director. When **S** is parallel to **L**, then **k** will also be parallel to **L**, with the electric field perpendicular to **L** ($n_{\text{eff}}=n_o$). When **S** is perpendicular to **L**, then **k** will also be perpendicular to **L**, with the electric field parallel to **L** ($n_{\text{eff}}=n_e$).

2.2 Static electric fields

The voltage in the LC layer will depend only on the z-coordinate, leading to a static electric field $\mathbf{E}^S$ along the z-axis, with amplitude depending on the orientation of the LC director. The magnitude of the electric field can be found from the charge density on the electrodes:

$$Q=\varepsilon_0\varepsilon_{zz}E_z^s=\varepsilon_0\left(\varepsilon_{\parallel}\cos^2\theta_L+\varepsilon_{\perp}\sin^2\theta_L\right)E_z^s$$
$$V_a=\int_0^d E_z^s dz=\int_0^d\frac{Q}{\varepsilon_0\left(\varepsilon_{\parallel}\cos^2\theta_L+\varepsilon_{\perp}\sin^2\theta_L\right)}dz \quad (9)$$

The electric field in the liquid crystal yields a torque which tries to align the liquid crystal with the electric field:

$$\Gamma_y^s=-\varepsilon_0\left(\varepsilon_{\parallel}-\varepsilon_{\perp}\right)\sin\theta_L\cos\theta_L E_z^{s2}$$
$$=-\frac{\left(\varepsilon_{\parallel}-\varepsilon_{\perp}\right)\sin\theta_L\cos\theta_L Q^2}{\varepsilon_0\left(\varepsilon_{\parallel}\cos^2\theta_L+\varepsilon_{\perp}\sin^2\theta_L\right)^2} \quad (10)$$

2.3 Elastic torques

In a one dimensional liquid crystal, the variation of the director in the xz-plane leads to an elastic torque, given by (assuming equal constants for splay and bend) [9]:

$$\Gamma_y^e = K \frac{\partial \theta_L^2}{\partial z^2} \tag{11}$$

2.4 Equilibruim LC director

When optic, electric and elastic torques act simultaneously on the liquid crystal, then the steady-state director distribution can be found by setting the sum of torques equal to zero:

$$\Gamma_y^o + \Gamma_y^s + \Gamma_y^e = 0$$

$$\tfrac{1}{2}\varepsilon_0\left(n_e^2 - n_o^2\right)\sin\left(\theta_L - \theta_S\right)\cos\left(\theta_L - \theta_S\right)E^2 - \varepsilon_0\left(\varepsilon_{\parallel} - \varepsilon_{\perp}\right)\sin\theta_L \cos\theta_L E_z^{s2} + K\frac{\partial\theta_L^2}{\partial z^2} = 0 \tag{12}$$

This is a differential equation in $\theta_L(z)$, equivalent to the equations in previous publications [3], but now extended to oblique incidence . The other variables can be eliminated, using the dependencies described above. The equation has to be completed with boundary conditions for the director orientation at $z=0$ and $z=d$. Hard boundary conditions refer to a fixed surface director: $\theta_L(0)=\theta_p$ and $\theta_L(d)=\theta_p$.

The liquid crystal director distribution in the LC layer depends not only on the electric field, but also on the light that passes through the liquid crystal. The dependency on the (intensity of the) light is a non-linear effect, for which intense laser beams are required. As the reorientation nonlinearity in liquid crystals is relatively strong (compared to other non-linear effects), the required intensity of the laser beam can be relatively modest.

If there is only an electrical field with planar alignment ($\theta_L=90°$), then the Freederickz transition voltage is given by the well known formula (mainly splay) [10]:

$$E_{TH}^s = \frac{\pi}{d}\sqrt{\frac{K_1}{\varepsilon_0\left(\varepsilon_{\parallel} - \varepsilon_{\perp}\right)}} \tag{13}$$

For E7, the threshold voltage $E_{TH}^s d$ is 0.96 Volt (using $K_1=12$pN).

In a similar way, the threshold for the optical field can be determined for perpendicular incidence of light $\theta_k=0°$, assuming that the director has the boundary condition $\theta_L=0°$ (vertically aligned). It should be noted that for small variations of the director, the Poynting vector deviates from the direction of the z-axis. The threshold for the electrical field and for the beam power are given by (in this case bend is most important):

$$E_{TH} = \frac{\pi}{d}\sqrt{\frac{2n_e^2 K_3}{\varepsilon_0 n_o^2\left(n_e^2 - n_o^2\right)}}$$

$$S_{TH} = \frac{c n_e^2 \pi^2 K_3}{n_o\left(n_e^2 - n_o^2\right)d^2} \tag{14}$$

This formula illustrates that the optical power threshold decreases with the square of the cell thickness. For a 100 μm thick device filled with E7, the threshold S_{TH} is about 18 W/mm^2 (using $K_3=18$pN). This means that intense laser light is needed in order to observe important effects of the optical fields.

2.5 Equilibrium LC director in a thick layer

For a sufficiently thick device, or for sufficiently strong static/optical electric fields, the torques in the bulk become negligible and the director orientation in the bulk can be calculated by setting the derivative with respect to z equal to zero. This leads to:

$$\frac{\sin(\theta_L-\theta_S)\cos(\theta_L-\theta_S)\sin\theta_k}{\cos(\theta_S-\theta_k)\cos\theta_S\sin\theta_L\cos\theta_L}=\frac{2(\varepsilon_{\parallel}-\varepsilon_{\perp})\tan\theta_m V_a^2}{(n_e^2-n_o^2)E_m^2 d^2} \qquad (15)$$

In this equation, θ_S can be eliminated by using:

$$\tan(\theta_L-\theta_S)=\frac{n_o^2}{n_e^2}\tan(\theta_L-\theta_k) \qquad (16)$$

and θ_k can be eliminated by using:

$$\frac{n_e n_o\sin\theta_k}{\sqrt{n_e^2\cos^2(\theta_L-\theta_k)+n_o^2\sin^2(\theta_L-\theta_k)}}=n_m\sin\theta_m \qquad (17)$$

Typically, there is one stable equilibrium director solution θ_{Lb} in the bulk (or equivalent $\theta_{Lb}+180^\circ$), which depends on the applied voltage V_a, the parameters of the incident beam and the properties of the LC.

In the absence of an optical field, an applied voltage will align the liquid crystal director along the z-axis: $\theta_{Lb}=0^\circ$ or $\theta_{Lb}=180^\circ$. In this case the denominators of the equations become zero.

In the absence of an electric field, the incident light will (in a sufficiently thick LC layer) align the director **L** perpendicular to the (**S**- and) **k**-vector and the effective index will be equal to n_e. In this case, the director orientation is given by:

$$\theta_L=\arcsin\left(\frac{n_m\sin\theta_m}{n_e}\right)\pm\frac{\pi}{2} \qquad (18)$$

This equation has a solution as long as the angle of incident light is sufficiently small. For $n_m\sin\theta_m>n_e$ light propagation in the liquid crystal becomes impossible.

2.6 Shift of the laser beam

The power of the laser beam travels along the Poynting vector. To find the horizontal shift of the laser beam during propagation through the LC layer, we have to integrate the x-component of the unit vector along the z-coordinate:

$$\Delta x=\int_0^d\tan\theta_S dz=\int_0^d\frac{n_e^2\tan\theta_L-n_o^2\tan(\theta_L-\theta_k)}{n_e^2+n_o^2\tan\theta_L\tan(\theta_L-\theta_k)}dz \qquad (19)$$

This illustrates that the lateral shift of the laser beam depends on the orientation of the liquid crystal.

3. SIMULATION RESULTS

All simulations are carried out for a cell thickness of 50 μm. The parameters for the liquid crystal are roughly the same as the commercially available LC E7 (Merck). The simulation parameters can be found in Table 1. The LC has nearly planar orientation near the surfaces, with a certain pretilt angle due to rubbing (2°). In the figures the tilt angle θ_T of the director is plotted (instead of the LC inclination angle $\theta_L = 90° - \theta_T$).

3.1 Numerical algorithm

In order to determine the steady state director distribution in a liquid crystal layer in the presence of an electric field and a light beam, equation (12) has to be solved, in combination with equations (16) and (17). We have written a simulation program in Matlab based on an iteration scheme, starting from an given initial condition. By starting from different initial conditions, different steady states may be found for the same applied voltage and/or incident light beam

Table 1. Important parameters used in the calculations (the liquid crystal used is E7).

Parameter	Value
$\varepsilon_{\perp}$	5.1
$\varepsilon_{//}$	19.6
n_e	1.7
n_o	1.5
K	12 pN

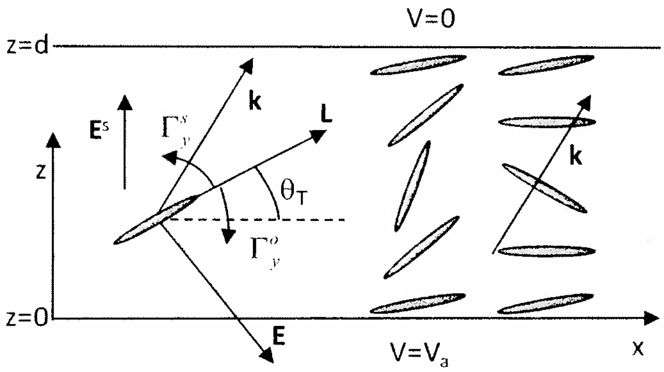

Fig. 2. Illustration of the torques due to the static electric field and the optical field, for a positive angle (left). Director distribution due to an applied voltage, indicated by the voltage V_a (middle, the tilt angle increases). Director distribution due to an optical field, indicated by the k-vector (right, the tilt angle becomes negative).

3.2 Influence of an applied voltage

In Fig. 3 the orientation of the director is shown for different applied voltages, for a cell with antiparallel rubbing. In this case, the y-axis is two-fold rotation axis and the tilt is symmetric with respect to $d/2$. The threshold voltage for the parameters of Table 1 calculated with equation (13) is 0.96 V. This value is compatible with the results in Fig. 3, as for 0.5 V and 0.8 V there is only a very small change in the tilt distribution. For higher voltages, the maximum tilt of the director increases and is close to 90° for high voltages.

Also visible in Fig. 3 is that there are two stable states for voltages of 1.0 V and higher. The state with positive tilt is energetically favorable and therefore a cell with antiparallel rubbing will always switch such that the tilt is in the same sense as the pretilt angle. The states with negative tilt are also stable at the appropriate voltages, but these states can only be obtained by applying additional electric or magnetic fields. For very high applied voltages, the mid-plane tilt will become nearly perpendicular (+90° or -90°) , as predicted by equation (15).

In Fig. 4 the director distribution is simulated for a similar case (only applied voltage), but now the cell has a +2° pretilt at one side an -2° pretilt at the other side. In practice this is realized by parallel rubbing of the alignment layers on the substrate. In this case the cell has mirror symmetry with respect to the xy-plane and the tilt versus x plot (Fig. 4) has inversion symmetry. In this case the state with positive tilt angle in the middle is equivalent in terms of energy to the state with negative tilt angle, because there is no preferential direction. It is clear that for low voltages – below the theoretical threshold for 0° pretilt – the absolute value of the tilt angle remains below 2°. For higher voltages the LC is forced into one of the two stable states with either predominantly positive or negative tilt angle. In practice, for parallel rubbed cells a non-uniform switching will be observed and such a LC cell will exhibit different domains. These domains are separated by domain walls [11].

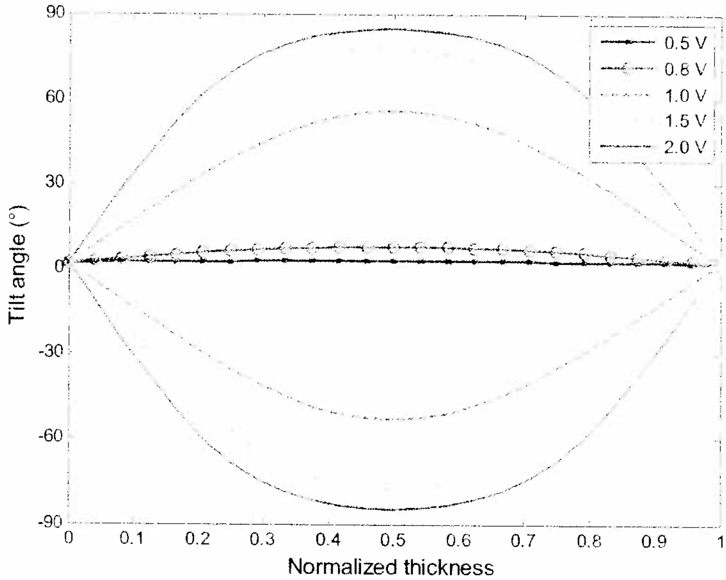

Fig. 3. Tilt angle distribution for different applied voltages, with pretilt angle +2° at both surfaces (antiparallel rubbing), no optical field is present. For the lowest voltages (0.5 V and 0.8 V) only one stable configuration can be found. For higher voltages two stable states are found (only the state with positive tilt is obtained by applying a voltage). The solutions are symmetric with respect to the middle of the cell.

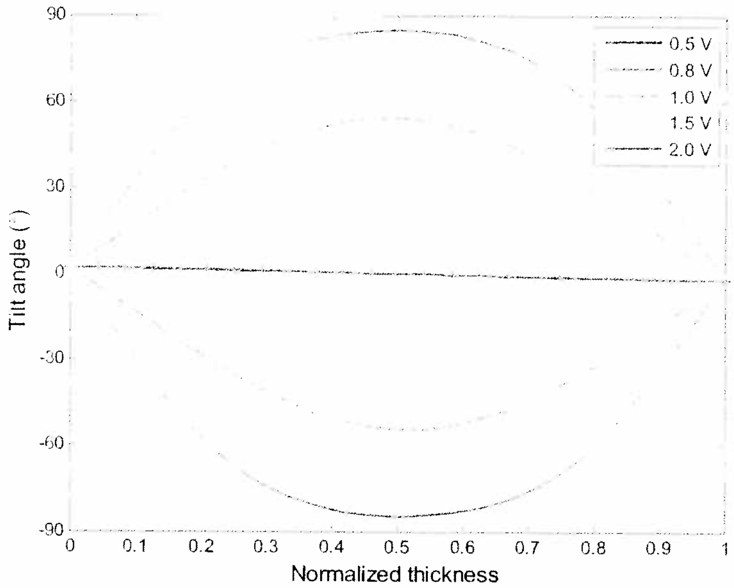

Fig. 4. Tilt angle distribution for different applied voltages (no optical field is present). The pretilt angle at the substrates is +2° and -2°. The solutions are antisymmetric with respect to the middle of the cell.

3.3 Influence of incident light

Fig. 5 gives the tilt angle distribution under influence of a plane wave incident from air, under an angle of 45°, in the absence of an applied voltage. The device has antiparallel rubbing (pretilt of 2° at both interfaces). Because the light has a positive inclination angle, the inclination angle of the electric field θ_E is larger than 90° and the tilt angle of the liquid crystal will decrease (as in the illustration of Fig. 2) and become negative if the intensity of the beam is sufficiently high. This means that the incident light can rotate the liquid crystal in a direction opposite to the rotation in the case of an applied voltage. For very high light intensities, the tilt of the liquid crystal in the middle of the device will saturate to the angle that corresponds to the formula in equation (15). Because the voltage is zero in this case, the asymptotic mid-plane tilt angle is found by setting the numerator of the left hand side equal to zero.

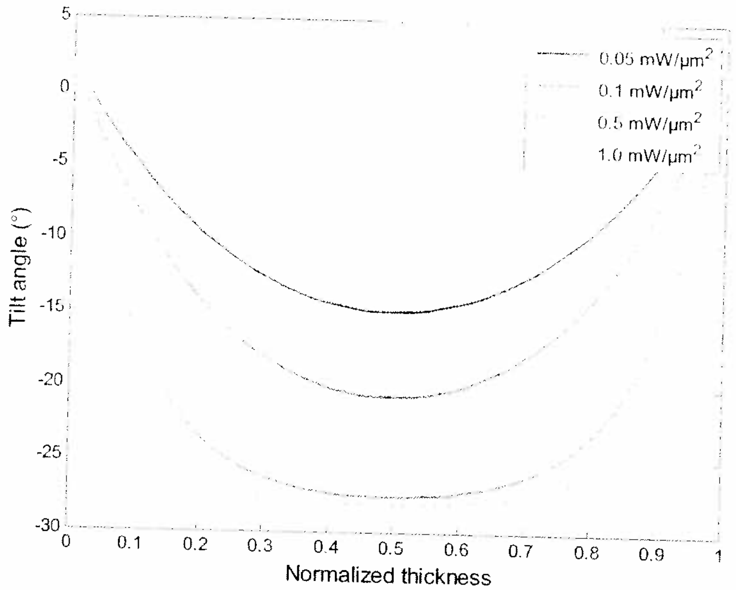

Fig. 5. Tilt angle distribution for an optical beam passing through the cell for different optical intensities. The angle from air of the optical beam is +45°. The pretilt angle is +2° at both boundaries. The solution is symmetric with respect to the middle of the cell.

The thickness of the device is 50μm, therefore, the with of the beam should be sufficiently large in order to achieve a homogeneous illumination over the entire thickness of the cell. If the area of illumination is smaller, the assumption of a one-dimensional structure is no longer satisfied, and the director calculations and the optical light propagation become more complicated, as in the case of soliton formation [4].

Fig. 6 shows the tilt angle distribution under influence of a plane wave incident from air, under an angle of -45°, in the absence of an applied voltage. The device has antiparallel rubbing (pretilt of 2° at both interfaces). In this case the inclination angle of the electric field θ_E in the liquid crystal is around 30° and the tilt angle of the liquid crystal will increase, similar to the case of applying a voltage.

Fig. 7 shows the tilt angle distributions for different angles of the incident light in air. The intensity of the light beam is sufficiently high, so that the liquid crystal director in the mid-plane aligns more or less parallel with the electric field of the incident light beam.

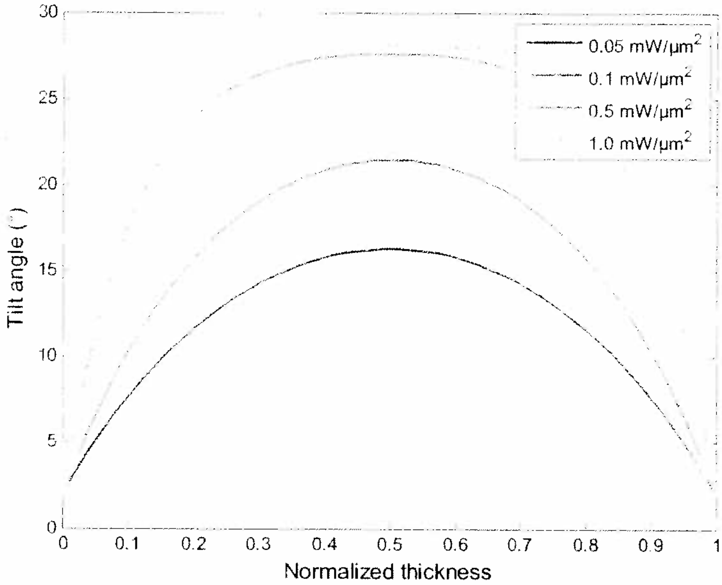

Fig. 6. Tilt angle distribution for an optical beam passing through the cell for different optical intensities. The angle from air of the optical beam is -45°. The pretilt angle is +2° at both boundaries.

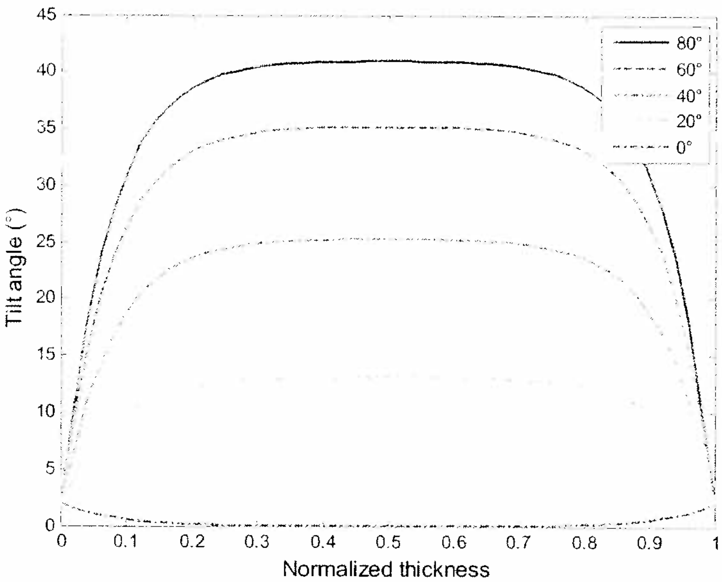

Fig. 7. Tilt angle for an optical beam passing through the cell at different angles (from air). The optical intensity is 1.0 $mW/\mu m^2$.

3.4 Combination of applied voltage and incident light

Fig. 8 finally illustrates the effect of combining the torques due to static and optical electric fields. As in the case of only an applied voltage, there are two stable states, one with positive and one with negative tilt. The important difference is now that both states can be accessed by applying the torques in the appropriate sequence.

When a voltage is applied starting from a homogeneous tilt of 2°, the tilt of the director will increase, similar as in Fig. 3. If the cell is then illuminated with light at an angle of 45°, the director orientation will then change only slightly until state 2 is reached. When the device is first illuminated under an angle of 45° in air, the director will tilt towards negative angles, similar to what happens in Fig. 5. In most of the device, the tilt angle is negative (only near the interfaces it is still positive), and therefore the torque due to an applied voltage will rotate the director further towards more negative angles. In this case the device will end up in state 1, with negative tilt angle.

If the incident light beam is switched of when the device is in state 1, the director will remain negative under influence of the applied voltage. This illustrates how the presence of illumination before the application of a voltage may cause the liquid crystal to switch to another stable state.

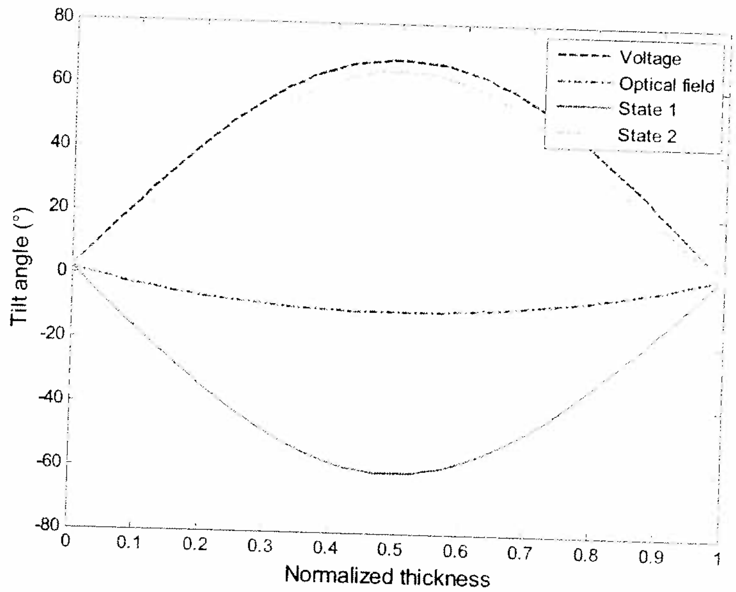

Fig. 8. Tilt angle for an applied voltage of 1.0 V (without optical field), for an optical field of 0.03 mW/μm^2 (zero voltage) and for the combination of both. State 1 and 2 denote the two stable states when both electric fields are present. The angle of the light beam in air is 45°.

3.5 Light path in the liquid crystal

According to equation (19) an incident beam will deviate depending on the tilt angle of the LC director. This is due to the longitudinal component of the anisotropy and this beam deviation has been experimentally observed in LC cells in different geometries [12-14]. As a first example the light path is calculated for a beam angle of 0° and very low optical intensity (see Fig. 9). The voltage is 1.0 V and 2.0 V and the cell thickness is 50 μm. Both the state with positive and negative tilt angle is illustrated. The deviation is either along the positive x-direction or the negative x-direction, depending on the sign of the tilt angle. The deviation angle from the z-axis is maximal for roughly 45° and minimum for 0° and 90° tilt angle [15]. This can also be seen in Fig. 9. For 2.0 V the deviation angle is small near the interfaces (because the pretilt angle is small, namely 2°) and in the middle of the cell (because the tilt angle is nearly 90°). The maximum deviation when reaching the second interface is 5 μm for 1.0 V.

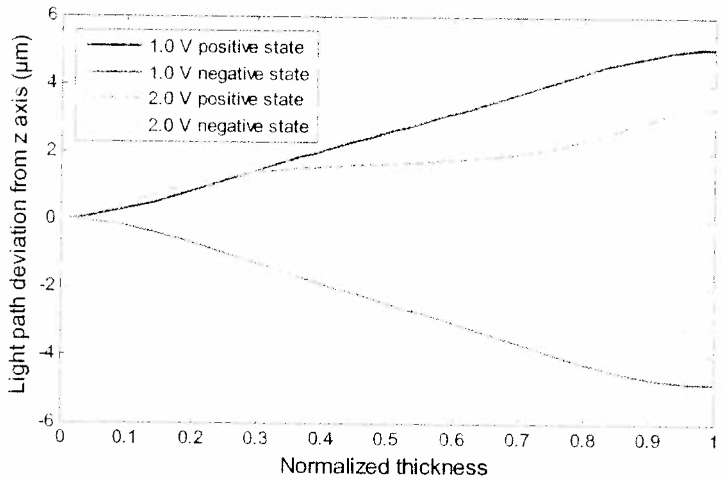

Fig. 9 Light path for an incident angle of 0° and an optical intensity close to zero. The parameters are the ones of Fig. 3 with a voltage of 1.0 V and 2.0 V. Both the state with positive tilt angle as the state with negative tilt angle is shown.

Fig. 10 shows the light path deviation from the z-axis for the two stable states that were found in Fig. 8. In this case the beam is propagating in the cell under a certain angle and the positive and negative state results in either an increase or a decrease of this angle. The difference in position at the second surface is more than 10 μm, so experimentally the two states should be distinguishable by measurement of the output position of the light beam.

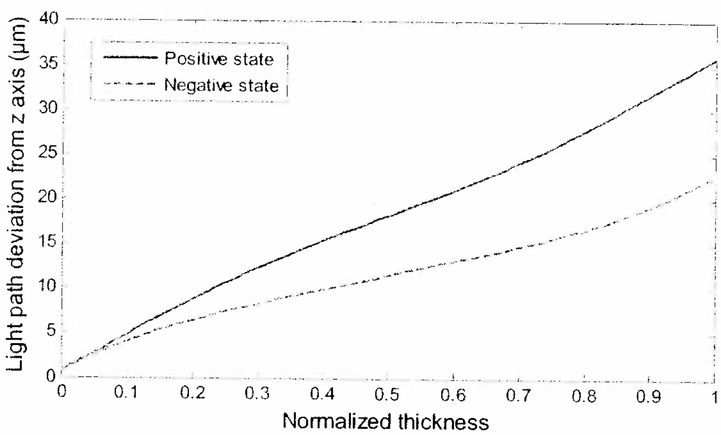

Fig. 10 Light path for an incident angle of 45° in air. The parameters are those used in Fig. 8.

4. CONCLUSION

In this manuscript we have presented theoretical considerations for the propagation of light beams in one-dimensional LC cells under oblique incidence. The liquid crystal orientation in these calculations depends on the applied voltage and the intensity of the light beam. This optical nonlinear effect leads to a set of nonlinear differential equations that have been solved numerically. Numerical examples show that an applied voltage can lead to two stable states of the liquid crystal orientation. With only voltage and no optical field only one of the two stable states can be obtained. In the presence of an obliquely incident light beam also the second stable state can be reached. Calculation of the light path inside the cell reveals that the two stable states can be distinguished by observing the beam position at the output side of the cell.

ACKNOWLEDGEMENTS

Jeroen Beeckman is postdoctoral fellow of the Research Foundation – Flanders (FWO). Wout De Cort is supported by the Institute for the Promotion of Innovation through Science and Technology in Flanders (IWT-Vlaanderen). This research has been carried out in the framework of the IAP project Photonics@be of the Belgian Science Policy and the FWO project 3G065609.

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PROCEEDINGS OF SPIE

Liquid Crystals XIII

Iam Choon Khoo
Editor

2-5August 2009
San Diego, California, United States

Volume 7414

SPIE

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Please use the following format to cite material from this book:
Author(s), "Title of Paper," in *Liquid Crystals XIII*, edited by Iam Choon Khoo, Proceedings of SPIE Vol. 7414 (SPIE, Bellingham, WA, 2009) Article CID Number.

ISSN 0277-786X
ISBN 9780819477040

Published by
SPIE
P.O. Box 10, Bellingham, Washington 98227-0010 USA
Telephone +1 360 676 3290 (Pacific Time) · Fax +1 360 647 1445
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