Simulation of 2-D lateral light propagation in nematic-liquid-crystal cells with tilted molecules and nonlinear reorientational effect

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Abstract. In the general case the optical tensor of a nematic liquid crystal consists of nine nonzero elements, which makes it difficult to calculate light propagation in a liquid-crystal cell. For a two-dimensional (2-D) problem with TM polarization and a parallel liquid-crystal orientation where the molecules are only tilted and not twisted, the full problem can be calculated by using one magnetic field component, thus reducing the problem to a scalar one. This geometry is used to simulate the self-focusing effect which can lead to the generation of spatial optical solitary waves. This self-focusing occurs due to the optical nonlinear effect of field-induced director reorientation. Due to nondiagonal elements of the optical tensor, however, it is expected that the Poynting vector will deviate from the original propagation direction. Our simulations reveal that, in this case, the deviation will not cause the loss of the soliton-like beam propagation regime, but will rather give rise to a transverse undulating behaviour.

Key words: beam-propagation method, liquid crystals, optical anisotropy, optical nonlinearity, spatial optical solitons

1. Introduction

Spatial optical solitons (SOS) are self-confined beams that propagate without diffraction. For the bright-soliton families, but without loss of generality, they can occur when the material has a nonlinear optical response that acts like a self-focusing – or self-lensing – mechanism for the light: when the self-focusing exactly balances the natural diffraction of the beam, a SOS is formed (Stegeman and Segev 1999). In optics they were first predicted to occur in nonlinear Kerr media (Ablowitz et al. 2000; Stegeman et al. 2000), but by now various kinds of SOS have been experimentally observed in different materials (Segev 1998). Recently, they have been observed in nematic liquid crystals (NLCs) owing to either a thermal nonlinear effect (Warenghem et al. 1998) or the nonlinear effect of optical field-induced director reorientation (Peccianti et al. 2000). In the latter case SOS can be observed with a few milliwatts of
light power and the propagation length can be as high as a centimetre, which is interesting for possible applications. Beyond this applied interest, however, the study of such narrow soliton-like beams generated via the molecular re-orientation of NLCs – sometimes called nematicons – led to a renewed fundamental interest in the field of SOS (Assanto et al. 2003). Such a consideration comes from the highly spatially nonlocal nature of the re-orientational nonlinearity of NLCs. Actually, the underlying theory of SOS in highly nonlocal nonlinear media is greatly simplified, as compared to those of local (Kerr-like) media, thus explaining why they are also called accessible solitons (Snyder and Mitchell 1997). In this connection, it appeared that nematicons are likely to be of accessible-soliton type, thus deserving a special attention (Conti et al. 2003). In this paper, we address the problem of considering the influence of the inherent optical anisotropy of a nematic liquid crystal on soliton-like light propagation in a planar-cell geometry. In previous works (Peccianti et al. 2000; Beeckman et al. 2003; Beeckman et al. 2004; Hutsebaut et al. 2004) the molecular orientation was modelled under the approximation of only one optical field component and the light propagation was simulated by a scalar beam-propagation method (BPM), hence neglecting the optical anisotropy of liquid crystals. Indeed, NLCs are uniaxial materials and, for an accurate description of the light propagation, a vectorial simulation method is desirable.

2. Geometry and orientation of the liquid crystal

Due to the one-dimensional orientational ordering in NLCs, the molecules have an average orientation defined by a vector called the director. In the experimental system, shown in Fig. 1 for the approximated 2-D geometry that we study in this paper, the nonlinear medium is a planar cell of nematic liquid crystal in parallel configuration [see (Peccianti et al. 2000; Beeckman et al. 2004; Hutsebaut et al. 2004) for details], NLC molecules are aligned by means of an alignment layer on the top and bottom glass plates that make up the cell. The molecules are then roughly aligned along the z direction as a slight tilt is introduced by the rubbing process. Because of this, in the absence of any electromagnetic field the molecules are uniformly oriented with a small angle of $\theta_0 = 2^\circ$ with respect to the z axis. A Gaussian laser beam is propagating laterally into the cell (i.e. initially in the z direction) with TM polarization, thus with a magnetic field along the y axis and an electric field mainly along the x axis.

A static electric field can be applied over the cell as the glass plates are covered with a thin electrode layer. The structure being invariant in the z direction, the static electric field has a component along the x axis only. This electric field induces a torque on the molecules because the static permittivity
of the NLC is anisotropic. Also, the optical electric field induces a torque on the molecules. The latter is similar to the torque induced by the static field, the optical anisotropy being now the determining factor. In order to obtain the stationary director orientation, one has to minimize the free energy of the system, the first part of which is the distortion free energy. In the case of Fig. 1, where the orientation of the director is described by the total reorientation angle $\theta$, the distortion free energy per unit volume can be written as:

$$f_d = \frac{1}{2} K \left( \frac{\partial \theta}{\partial x} \right)^2.$$  \hfill (1)

The $y$-derivative is zero because of the considered 2-D geometry, and the $z$-derivative is neglected because it is assumed that variations along $z$ are slow. Furthermore, formula (1) assumes the usual hypothesis of equal values of the Frank constants of splay and bend [i.e. $K_1 = K_3 = K$, the value for the constant of twist ($K_2$) being here of no importance as there is no such molecular motion for this specific situation (Gennes and Prost 1993)]. The second part of the free energy is the energy arising from the static and optical electric fields, given respectively by

$$f_s = -\frac{1}{2} E_s^s \cdot \bar{\varepsilon} \cdot E^s,$$  \hfill (2a)

$$f_o = -\frac{1}{2} E_o^o \cdot \bar{\varepsilon} \cdot E^o.$$  \hfill (2b)

In these formulas the permittivity tensor is of the form:

$$\bar{\varepsilon} = \varepsilon_0 \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xz} \\ \varepsilon_{zx} & \varepsilon_{zz} \end{bmatrix} = \varepsilon_0 \begin{bmatrix} \varepsilon_{\perp} + \Delta \varepsilon \sin^2 \theta & \Delta \varepsilon \sin \theta \cos \theta \\ \Delta \varepsilon \sin \theta \cos \theta & \varepsilon_{\perp} + \Delta \varepsilon \cos^2 \theta \end{bmatrix}.$$  \hfill (3)

To minimize the total free energy, the Euler–Lagrange formula is used (Gennes and Prost 1993). Taking into account that the static electric field

Fig. 1. Geometry and axes.
has a component in the $x$ direction only whereas the optical electric field has both an $x$- and a $z$-component, one finds the following differential equation:

$$
K \frac{\partial^2 \theta}{\partial x^2} + \frac{1}{2} \epsilon_0 \Delta \epsilon \sin 2\theta |E^s|^2 \\
+ \frac{1}{2} \epsilon_0 \Delta \epsilon \sin 2\theta (|E_x^o|^2 - |E_z^o|^2) + \cos 2\theta (E_x^o E_z^o + E_z^o E_x^o) = 0.
$$

This differential equation is solved numerically by using a relaxation method (Press et al. 1992). In this formula, the static field has to be adapted for the changed permittivity when the molecules reorient. The static electric field has to fulfil the Maxwell’s equation $\nabla \cdot (\overrightarrow{\epsilon} \cdot \overrightarrow{E}) = 0$, which can be reduced to the following condition:

$$
E^s = \text{constant} \frac{\overrightarrow{\epsilon}^s}{\epsilon_\perp + \Delta \epsilon \sin^2 \theta}.
$$

In the following sections, when we mention the optical field and optical dielectric tensor the superscript ‘o’ is omitted for the sake of simplicity.

### 3. Transmission and reflection of a plane wave at the air–NLC interface

In Fig. 2 an incoming plane wave with wave vector $\vec{k}_i$ reaches the air–NLC interface. Part of the light is reflected whereas the other part is transmitted. When the light power is increased the NLC molecules reorient, which implies that the reflection and transmission coefficients change. To give an idea of these coefficients, the situation of Fig. 2 is considered. When $\vec{k}_i$ is oriented along the $z$ axis, the transmitted and reflected wave vectors will also have a $z$-component only. The value for the transmitted wave vector has to be calculated from the following condition for wave vectors in uniaxial materials (Yeh and Gu 1999):

$$
(k_z^2 - k_0^2 \epsilon_{xx}) k_0^2 \epsilon_{zz} + (k_0^2 \epsilon_{zz})^2 = 0,
$$

with the wave number in vacuum denoted as $k_0$. The electric fields of the incoming and reflected waves have an $x$-component only, while the transmitted field has both an $x$- and a $z$-component. Using $\vec{H} = (j/\omega \mu_0) \nabla \times \overrightarrow{E}$ and applying the boundary conditions, i.e. the continuity of the tangential components of the magnetic and electric fields, the following relationships between incoming and transmitted fields can be found:
The wave vector for the transmitted plane wave lies along the \( z \) axis and the magnetic field along the \( y \) axis, but the electric field is not perpendicular to the wave vector any more. As a result, the Poynting vector \( \vec{E} \times \vec{H} \) is also not along \( z \). This means that the direction of the flow of optical energy can vary due to a director variation of the liquid crystal. The angle \( \varphi \) between the direction of the energy flow and the \( z \) axis is given by

\[
\tan \varphi = \frac{E^t_y}{E^t_x} = \frac{\varepsilon_{yz}}{\varepsilon_{zz}} \frac{\Delta \varepsilon \sin \theta \cos \theta}{\varepsilon_{zz} + \Delta \varepsilon \cos^2 \theta}.
\]

(8)

Figure 3 shows the dependency of the molecular tilt on this angle, for the parameters of a typical NLC [E7 from Merck with \( \Delta \varepsilon = 0.743 \) and \( \varepsilon_{zz} = 2.320 \) (Yeh and Gu 1999)]. The maximal deviation angle of about 8° is obtained for a tilt of about 49°. The following simulation results will illustrate the influence of this effect on soliton-like propagation in NLCs.
4. 2-D vectorial beam-propagation method

To develop a BPM for the described geometry, we start from Maxwell’s equations for the optical electric and magnetic fields. These equations are applied to the 2-D situation, independent of \( y \), of Fig. 1. The electric field has components along \( z \) and \( x \), but the magnetic field has a component along \( y \) only. Therefore, it is convenient to eliminate the electric field components and to write the equations in function of the magnetic field. To do so, we need the inverse matrix of \( \vec{\varepsilon} \). For ease of notation, we will write this matrix as follows:

\[
\vec{\varepsilon}^{-1} = \frac{1}{\varepsilon_{xx}\varepsilon_{zz} - \varepsilon_{xz}^2} \begin{bmatrix} \varepsilon_{zz} & -\varepsilon_{xz} \\ -\varepsilon_{xz} & \varepsilon_{xx} \end{bmatrix} \begin{bmatrix} \tilde{e}_{xx} & \tilde{e}_{xz} \\ \tilde{e}_{xz} & \tilde{e}_{zz} \end{bmatrix}.
\] (9)

With these assumptions we can write the Maxwell’s equations as:

\[
\begin{bmatrix} E_x \\ E_z \end{bmatrix} = jk \begin{bmatrix} \tilde{e}_{xx} & \tilde{e}_{xz} \\ \tilde{e}_{xz} & \tilde{e}_{zz} \end{bmatrix} \begin{bmatrix} \frac{\partial H_y}{\partial x} \\ \frac{\partial H_y}{\partial z} \end{bmatrix},
\] (10a)

\[
\frac{\partial E_x}{\partial z} - j\omega \mu_0 \varepsilon_0 H_z = \frac{\partial E_z}{\partial x}.
\] (10b)

Eliminating \( E_x \) and \( E_z \) then gives

\[
k_0^2 H_y = \left( \frac{\partial e_{zz}}{\partial z} - \frac{\partial e_{xz}}{\partial x} \right) \frac{\partial H_y}{\partial x} + \left( \frac{\partial e_{xz}}{\partial x} - \frac{\partial e_{xx}}{\partial z} \right) \frac{\partial H_y}{\partial z} + 2 \frac{\partial^2 H_y}{\partial x \partial z} - \tilde{e}_{xx} \frac{\partial^2 H_y}{\partial z^2} - \tilde{e}_{zz} \frac{\partial^2 H_y}{\partial x^2}.
\] (11)

It can be seen that, for this specific situation, the problem can be reduced to a scalar one. A similar scheme is applied in (Kriezis and Elston 1999) for the simulation of light propagation in displays, under a wide-angle approximation. This equation is then further transformed by assuming paraxiality of the optical magnetic field. We write \( H_y(x, z) = H_Y(x, z) \exp(-j k z) \) and we neglect the terms with the second derivatives of \( H_Y \) in \( z \) with respect to the other terms. This approximation is valid when the propagation angle of the light with respect to the \( z \) axis is limited to a few degrees and when the medium exhibits moderate contrast in its optical properties (Hadley 1992a). Finally, this results into
\[
A_1 \frac{\partial^2 H_y}{\partial x \partial z} + A_2 \frac{\partial H_y}{\partial z} = B_1 H_y + B_2 \frac{\partial H_y}{\partial x} + B_3 \frac{\partial^2 H_y}{\partial x^2},
\]
with coefficients
\[
A_1 = 2\overline{e}_{xz},
A_2 = \frac{\partial \overline{e}_{xz}}{\partial x} - \frac{\partial \overline{e}_{xx}}{\partial z} + 2jk\overline{e}_{xx},
B_1 = k_0^2 + jk \left( \frac{\partial \overline{e}_{xz}}{\partial x} - \frac{\partial \overline{e}_{xx}}{\partial z} \right) - k^2 \overline{e}_{xx},
B_2 = \frac{\partial \overline{e}_{xz}}{\partial x} - \frac{\partial \overline{e}_{zz}}{\partial z} + 2jk\overline{e}_{zz},
B_3 = \overline{e}_{zz}.
\]

From these formulas, the propagation along the z axis can be calculated by applying a finite-difference scheme, resulting in the solution of a tridiagonal matrix when z-derivatives of the $\overline{e}$-matrix elements are neglected. In the case of an isotropic material the equations reduce to the simple scalar finite-difference BPM, as for example in (Chung and Dagli 1990). Transparent boundary conditions are used (Hadley 1992b).

When including the reorientational nonlinear effect, described in Section 2, the algorithm is as follows (see Fig. 4). The values of the magnetic field at $z = (n + 1)\Delta z$ are calculated from the magnetic field at $z = n\Delta z$ and the director orientation in the middle. From the magnetic fields in these two layers, the electric fields in the middle are calculated – according to (10) – and with these values the director orientation is recalculated. This procedure is repeated until consistency and desired accuracy is achieved, and before going on to the next step of calculation. For typical parameters of the simulation, 1–5 iterations are necessary to obtain an accurate value of $\theta$.

5. Simulation results

5.1. Test of simulation method for a NLC waveguide

For a glass–NLC–glass waveguide with uniformly tilted molecules, guided modes can be calculated analytically. An optical beam injected in this waveguide couples to one of these modes after a sufficient propagation distance. Figure 5 shows the evolution of the optical field amplitude along the propagation distance for a Gaussian beam injected in the NLC waveguide. The plots on the right show that, after a propagation distance of 800 μm, the
central beam profile matches the analytically calculated mode profile of the single-mode waveguide, which proves the validity of the derived BPM. Note that, in this case, there is no optically induced molecular reorientation, i.e. a linear propagation regime is considered for the purpose of the test.

5.2. SPATIAL SOLITONS IN A BULK NLC LAYER

When applying a voltage over a cell, molecules tilt due to the torque of the electric field. At the borders of the cell, the molecules keep their original orientation, imposed by the alignment layers (see Fig. 6). Because of this, the light propagating laterally in the cell will see a bigger index of refraction in the middle of the layer. When an optical field is present, its electric field component also gives rise to a torque equation (4) and the molecules tilt more and, consequently, the index of refraction increases again. When the director orientation is horizontal or vertical, the torque on the molecules is zero. The maximal torque corresponds to an orientation of about 45° with respect to the z axis. By tilting the molecules a little (using a voltage below the threshold) the optical nonlinear effect can be enhanced significantly.
For the same reason, a small pretilt of the molecules at the border is used. As highlighted in Section 3 for the specific case of a plane wave propagating in a bulk NLC, we are here interested in showing how the off-axis deviation of the beam, due to the anisotropy, affects the possible generation and propagation of a soliton. The simulations were performed for the parameters of the NLC E7 from Merck, as mentioned before. The thickness of the cell is 75 μm and the optical beam is a Gaussian beam with a waist of 3 μm and a wavelength of 980 nm. The optical power is expressed in mW/μm in the y direction. In Figs. 7b–f light propagation through the cell is shown for a beam launched at normal incidence with respect to the input (Fig. 7a). For 0 V over the cell (Fig. 7b), the beam is spreading out due to the predominant diffraction, together with a slight deviation caused by the small pretilt of the molecules. When 1 V is applied over the cell (Figs. 7c–f), the beam deviates more, in accordance with an increased molecular orientation. However, the simulation reveals that the light does not exit the cell, but reflects back toward its centre. Indeed, because of the vicinity of the glass–NLC interface, where molecular orientation is fixed by the rubbing, light encounters a stronger and stronger refractive-index gradient that is able to reflect the beam, which subsequently undergoes another deviation regime until the opposite interface. [For lower voltages (not shown), the light exits the cell because the index gradient is not strong enough to keep the light in the cell.] As a result, the joint effects of strong enough field-induced molecular orientation at the centre of the cell (causing beam deflection) and refractive-index gradient imposed by the hard boundary conditions (causing beam reflection) are responsible for a periodic transverse undulation of light during propagation. In addition, when the optical field power is increased, the nonlinear self-focusing effect confines the beam more and more (Figs. 7d–f). For a certain value of power (Fig. 7f), the beam width remains approximately constant along with the propagation distance, which features a soliton-like propagation regime. It is nevertheless not a strict soliton.
behaviour because of the transverse undulation of the beam. However, these simulations show that the deviation of the flow of optical power due to the anisotropy is expected not to prevent the stability of the soliton-like behaviour. Also, it is worth mentioning that the beam width is not strictly invariant but rather oscillating, each extremum of the undulation corresponding to a maximum of beam width. Also from Fig. 7, it can be seen that the characteristic length of undulation shortens with increasing optical field. This is because the tilt distribution is situated in a region where the deviation angle increases with increasing tilt angle ($\theta < 49^\circ$ according to Fig. 3). For these simulations the maximal off-axis propagation angle is close to $8^\circ$ and the maximal permittivity contrast $\Delta\varepsilon/\varepsilon$ is about 0.13 for a tilt angle of $40^\circ$ (see Fig. 6). In (Hadley 1992a) it is shown that for these values the relative error introduced by the paraxial scheme is of the order of a few percents and therefore acceptable.

In order to avoid the undulation of the beam, one could launch it under a certain angle with respect to the $z$ axis. Figure 8 shows that the amplitude of undulation indeed becomes much smaller, suggesting that it could be almost inhibited provided that an appropriate angle of incidence is chosen. Finding the appropriate angle, however, is somewhat empirical. Moreover, for each parameter (voltage, optical power ...), this angle changes so that it is difficult to avoid the beam undulation, which can be a major drawback for future applications.

Finally, we would like to mention that beam undulation has already been observed in parallel NLCs in a cylindrical geometry which, under a 2-D approximation, reduces to the problem studied here but without any static

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**Fig. 7.** (a) Schematic view of the simulation geometry and orientation of molecules when applying 1 V over the cell. (b-f) Optical field amplitude of light propagating in the cell: (b, c) for 0 V and 1 V respectively with very low optical power; (d–f) for 1 V with increasing optical power, respectively 0.03, 0.11, and 0.24 mW/µm. (Note that the scales for $x$ and $z$ directions are different.)
electric field. In (Braun et al. 1993) undulation was hence observed at high optical powers and intuitively explained on the basis of our same consideration of light propagation in uniaxial birefringent crystals, whereas in (McLaughlin et al. 1996) the effect was described by an analytical model.

6. Conclusion

The simulation method reveals features of the soliton propagation in NLCs which cannot be explained by a scalar method. To our best knowledge, we believe that the present work, besides the benefit of having a numerical simulation at our disposal, is original, as our results provide new insights into those phenomena related to soliton-like light propagation in NLCs. It is shown that, when entering the cell, the beam exhibits off-axis deviation due to the anisotropy of the tilted molecules. Such a behaviour can be anticipated from geometrical ray optics of uniaxial crystals. This deviation, however, does not prevent the possibility of a soliton-like propagating mode in which the beam evolves with a nearly constant width. Furthermore, such a deviation of the soliton-like beam leads to its transverse undulation, the amplitude and period of which depend on parameters such as applied voltage and optical power. These results suggest that narrow SOS generated in nematic-liquid-crystal planar cells should undulate across the thickness of the cell as they propagate. Experimental work is currently under investigation in order to observe this behaviour.

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References