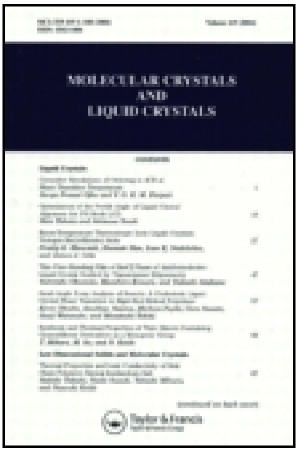

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Modeling of Nonlinear Beam Propagation in Chiral Nematic Liquid Crystals

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In this work three dimensional full-vector beam propagation method derived directly from Maxwell equations and combined with the exact equations describing director reorientation are presented. Molecules reorientation model bases on the Frank-Oseen equation with two angles (twist and azimuthal) describing molecule orientation. Solutions of light propagation in chiral nematic liquid crystals for different input beam polarization are shown. Formation of a soliton-like beam which has been already observed in many experiments is analyzed. Comparison between two-angle model and one-angle model assuming reorientation in a single plane is also provided.

Keywords Chiral nematic liquid crystals; cholesterics; full-vector beam propagation method; light propagation; nematicons; spatial solitons

Introduction

Chiral nematic liquid crystals are unique materials in nonlinear optics due to their vast reorientational nonlinearity and anisotropy. As the director orientation changes along the structure, modeling of molecules reorientation and light propagation require vectorial methods. At first some general work and analytical description of liquid crystal molecules reorientation have been done by Friedel [1] and Oseen [2] and later extended by Frank [3]. Some effort have been made to describe light propagation in chiral [4] and non-chiral [5] nematics using analytical approach. Development of Beam Propagation Method (BPM) in 1976 by Fleck and Feit [6] made it possible to describe light propagation more accurately. At next many numerical methods and approaches have been developed when it comes to beam propagation method [7] and molecules reorientation in liquid crystals [8]. As well chiral as non-chiral nematics were applied to develop displays [9, 10]. In recent years soliton-like beam formation was observed and studied in nematics by numerous scientific groups [11–15]. Some work describing soliton steering [16–18] and soliton iteractions [19, 20] in non-chiral nematics has been already made. When it comes to numerical simulations of chiral nematics simple linear vectorial analysis have been made [21]. In this work Full-Vector Beam Propagation Method (FV-BPM) combined with molecules reorientation model to describe light propagation in chiral nematic liquid crystals is presented. In our simulations not only twist reorientation is taken into account as it was made in previous works but also azimuthal reorientation. Differences between exact approach (two-angle model) and

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that assuming reorientation only in a single plane (one-angle model) are discussed. Light propagation with detailed look at the polarization, width and shape of the propagated beam is presented.

Beam Propagation Method

Chiral nematic liquid crystals (ChNLCs) are anisotropic medium and their molecules director changes along the structure. For this reason use of vectorial methods is required. In this work FV-BPM derived directly from two following Maxwell equations is used:

$$\nabla \times \vec{E} = -\mu\mu_0 \frac{\partial \vec{H}}{\partial t}$$
$$\nabla \times \vec{H} = \varepsilon\varepsilon_0 \frac{\partial \vec{E}}{\partial t} \tag{1}$$

It is assumed that electric and magnetic fields are complex which leads to six partial differential equations of the form:

$$\begin{aligned}
\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} &= i\omega_0\varepsilon_0\left(\varepsilon_{11}E_x + \varepsilon_{12}E_y + \varepsilon_{13}E_z\right)\\
\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} &= i\omega_0\varepsilon_0\left(\varepsilon_{21}E_x + \varepsilon_{22}E_y + \varepsilon_{23}E_z\right)\\
\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} &= i\omega_0\varepsilon_0\left(\varepsilon_{31}E_x + \varepsilon_{32}E_y + \varepsilon_{33}E_z\right)\\
H_x &= -\frac{1}{i\mu_0\omega_0}\cdot\left(\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z}\right)\\
H_y &= -\frac{1}{i\mu_0\omega_0}\cdot\left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x}\right)\\
H_z &= -\frac{1}{i\mu_0\omega_0}\cdot\left(\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}\right)
\end{aligned} \tag{2}$$

where ε_{mn} is a component of the electric permittivity tensor. Subsequently equations (2) are rewritten using symmetric finite differences and solved using 4^{th} order Runge-Kutta method.

Molecules Reorientation Model

For detailed description of light propagation in liquid crystals it is crucial to simulate molecules reorientation which is an important source of nonlinearity in ChNLCs. We use coordinate system shown in Fig. 1. We startup with Frank-Oseen equation on free energy density:

$$f = \frac{1}{2}K_{11}\left(\nabla\vec{n}\right)^2 + \frac{1}{2}K_{22}\left(\vec{n}\cdot(\nabla\times\vec{n}) - G\right)^2 + \frac{1}{2}K_{33}\left(\vec{n}\times(\nabla\times\vec{n})\right)^2 +$$
$$-\frac{1}{2}\Delta\varepsilon\varepsilon_0\left(\vec{n}\cdot\vec{E}\right)^2 \tag{3}$$

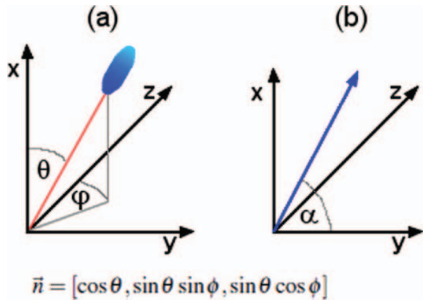

Figure 1. Coordinate system for (a) molecules orientation and (b) polarization angle.

where $\Delta\varepsilon = \varepsilon_{||} - \varepsilon_{\perp}$—electric anisotropy, $\varepsilon_{||}, \varepsilon_{\perp}$—correspond to the extraordinary and ordinary electric permittivity respectively. Parameter $G = 2\pi/p$, (where p-pitch) describes liquid crystals chirality. Director $\vec{n}$ is defined as follows:

$$\vec{n} = [\cos\theta; \quad \sin\theta\sin\varphi; \quad \sin\theta\cos\varphi]$$

Molecules deformations are described by three Frank elastic constants: K_{11} (splay), K_{22} (twist) and K_{33} (bend). To simplify the calculations we make often used assumption [22] that all elastic constants are equal $K_{11} = K_{22} = K_{33} = K$. Although for the simulated liquid crystal it is true that $K_{11} \approx K_{33}$ assuming $K_{11} \approx K_{22}$ and $K_{22} \approx K_{33}$ may introduce quantitive inaccuracies. However, in some configurations (for instance for y-polarized light) only twist deformation plays a crucial role. In such a case single constant approximation gives also quantitively correct results.

Next we substitute equation (3) into Euler-Lagrange equations:

$$\begin{aligned} \frac{\partial}{\partial x}\frac{\partial f}{\partial \varphi_x} + \frac{\partial}{\partial y}\frac{\partial f}{\partial \varphi_y} - \frac{\partial f}{\partial \varphi} = 0 \\ \frac{\partial}{\partial x}\frac{\partial f}{\partial \theta_x} + \frac{\partial}{\partial y}\frac{\partial f}{\partial \theta_y} - \frac{\partial f}{\partial \theta} = 0 \end{aligned} \tag{4}$$

where θ_x, φ_x, φ_y, θ_y—derivatives with respect to x and y. Two two-dimensional partial differential equations describing twist and azimuthal reorientation are obtained. Next they are solved using Successive Over-Relaxation (SOR) method [23] with relaxation parameter less than one, so actually under-relaxation is used. Obtained $\theta(x, y)$ and $\varphi(x, y)$ distributions are substituted into permittivity tensor of the form:

$$\varepsilon = \begin{bmatrix} \varepsilon_{\perp} + \Delta\varepsilon\cos^2\theta & \Delta\varepsilon\sin\theta\cos\theta\sin\varphi & \Delta\varepsilon\sin\theta\cos\theta\cos\varphi \\ \Delta\varepsilon\sin\theta\cos\theta\sin\varphi & \varepsilon_{\perp} + \Delta\varepsilon\sin^2\varphi\sin^2\theta & \Delta\varepsilon\sin\varphi\cos\varphi\sin^2\theta \\ \Delta\varepsilon\sin\theta\cos\theta\cos\varphi & \Delta\varepsilon\sin\varphi\cos\varphi\sin^2\theta & \varepsilon_{\perp} + \Delta\varepsilon\sin^2\theta\cos^2\varphi \end{bmatrix}$$

Such a tensor is used in FV-BPM in equation (2). When assuming that reorientation occurs only in yz plane and that $\theta(x, y) = \frac{\pi}{2}$ equation can be simplified and rewritten as:

$$\frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} + \frac{\Delta\varepsilon\varepsilon_0}{2K_{22}}\left[2E_yE_z\cos(2\varphi) + (|E_y|^2 - |E_z|^2)\sin(2\varphi)\right] = 0 \tag{5}$$

Although in equation (5) there is no parameter G which vanishes right after assuming $\theta(x, y) = const$. it describes as well chiral and non-chiral nematics. Equation (5) has many solutions but only one that minimizes equation (3) gives the right result.

Numerical Results

Numerical simulations were performed in (2+1)D case on a transverse grid of 200×200 points. Integration steps were set as follows: $\Delta x = \Delta y = 0.25\,\mu$m. Light was propagated along the z-axis at a distance of 1000 μm with a step $\Delta z = 0.01\,\mu$m. The cell was 50 μm in height (see Fig. 2). At the boundaries Dirichlet conditions were used. Pitch of a cholesteric was set to $p = 25\,\mu$m.

Molecules reorientation was recalculated after each 0.5 μm of propagation. A Gaussian beam of a wavelength $\lambda = 793$ nm was launched into the system. Parameters of the liquid crystal correspond to the nematic liquid crystal 6CHBT ($n_e = 1.6714$, $n_o = 1.5144$, $K = 3.7\,pN$).

At first simulations presenting soliton-like beam formation were performed (see Fig. 3). Input beam polarization was set along the y axis ($\alpha = 0°$). Such non-diffractive beam was observed as well for the beam launched at the center as for the beam launched slightly below the center ($\Delta x = 2\,\mu$m). Minimum input beam power to form soliton-like beam was respectively $P_{\min}(\Delta x = 0\,\mu\text{m}) = 10$ mW and $P_{\min}(\Delta x = 2\,\mu\text{m}) = 45$ mW. Beam launched directly at the center was propagated straight along the z axis in contrast to the beam launched Δx = 2 μm below the center which tended to go off-axis and showed shift of approximately Δy = 5 μm from the center at z = 1000 μm. Note that some part of the energy was diffracted sideways at the input (Fig. 3(a)). Then it went back to the center of the cell which is a numerical effect caused by Dirichlet boundary conditions. This part of energy is weak and does not significantly affect soliton-like beam formation.

Subsequently simulations using two-angle model were compared with those assuming reorientation only in yz plane (one-angle model). Beam shape and FWHM at the output in function of polarization for a beam of P = 60 mW launched 2 μm below the center, are shown in Fig. 4.

For polarization angles close to the y axis ($\alpha < 30°$) differences in shape and beam width are negligible which means one-angle model is sufficient enough for simulating light propagation. For polarization angles further from the y axis ($\alpha \geq 30°$) differences become evident in beam shape, intensity and even output position. Using one-angle model results in a stronger shift of the beam from the center. Polarization distribution and light intensity for

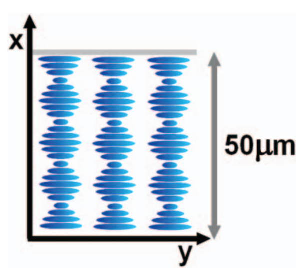

Figure 2. Schematic drawing of the ChNLC cell.

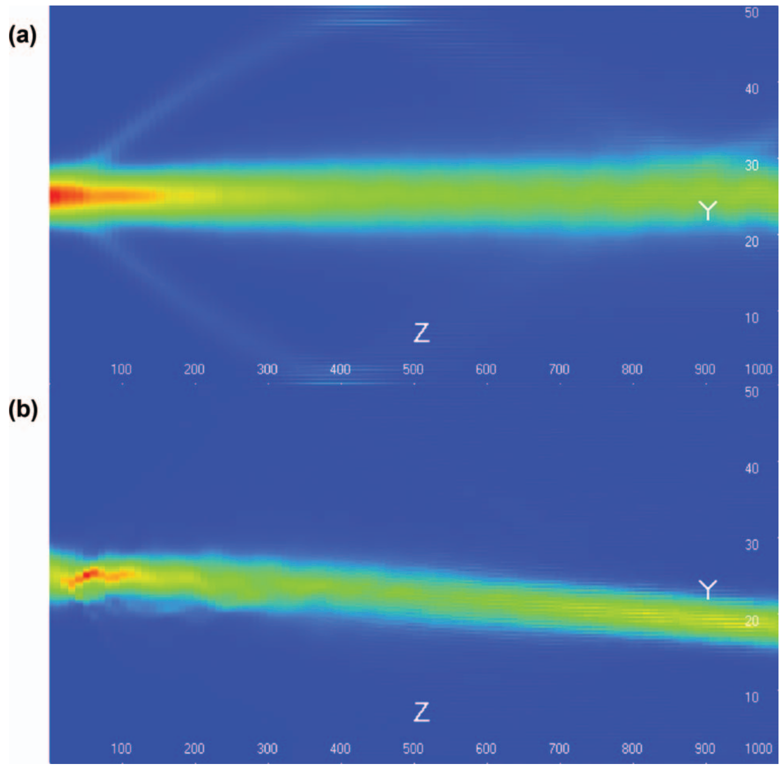

Figure 3. Sum (along the x-axis) of light intensity in yz plane. Soliton-like beam is observed for (a) input beam power P = 10 mW and launched at the center and for (b) input beam power P = 45 mW launched $\Delta x = 2\,\mu$m below the center. Input polarization is along the y-axis ($\alpha = 0^\circ$).

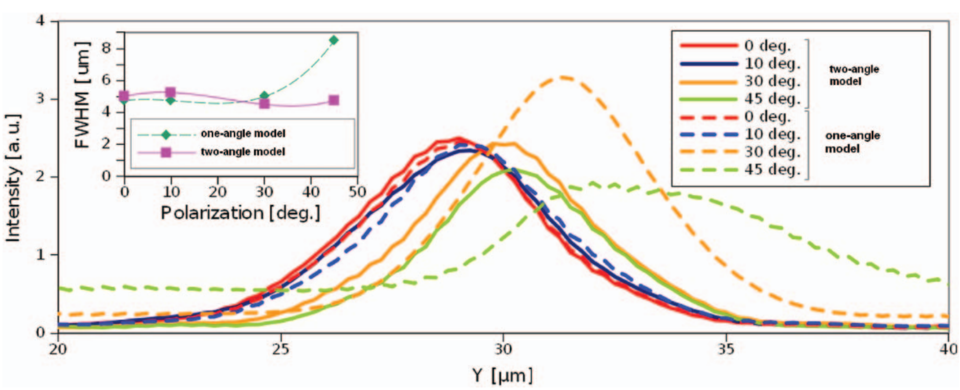

Figure 4. Intensity distribution of the beam cross section at $z = 1000\,\mu$m for P = 60 mW and beam launched 2 um below the center. FWHM in function of polarization is shown in the upper left corner.

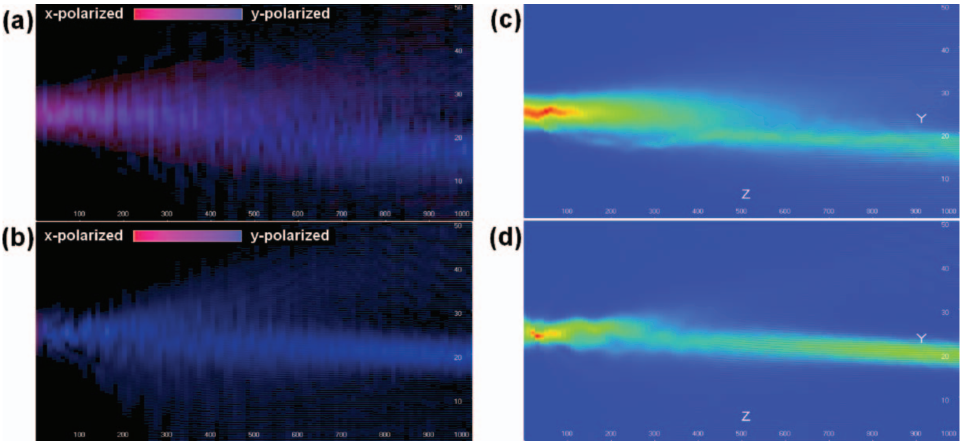

Figure 5. Polarization distribution (left) and light intensity distribution (right) for the input power P = 60 mW and beam polarized at $\alpha = 45^\circ$ launched $\Delta x = 2\,\mu$m below the center. Calculations performed using one-angle model (a)(c) and two-angle model (b)(d).

the polarization $\alpha = 45^\circ$ are shown in Fig. 5. Assuming that reorientation occurs only in yz plane we observe that x-polarized light is fully diffracted. For the exact, two-angle model some part of the x-polarized light is changed into y-polarized light and the rest is strongly diffracted. It explains different power values needed for soliton-like beam formation. In Fig. 6 it is clearly visible that output beam shape and width are different. Moreover in two-angle model as the beam goes off-axis, x-polarized light only weakly destabilizes the soliton-like beam.

At next, beams launched at the center of the cell were compared. Simulations were performed for P = 30 mW and polarization angle $\alpha = 45^\circ$ (see Fig. 7). Polarization distributions are also different but this time assuming reorientation only in yz plane leads to

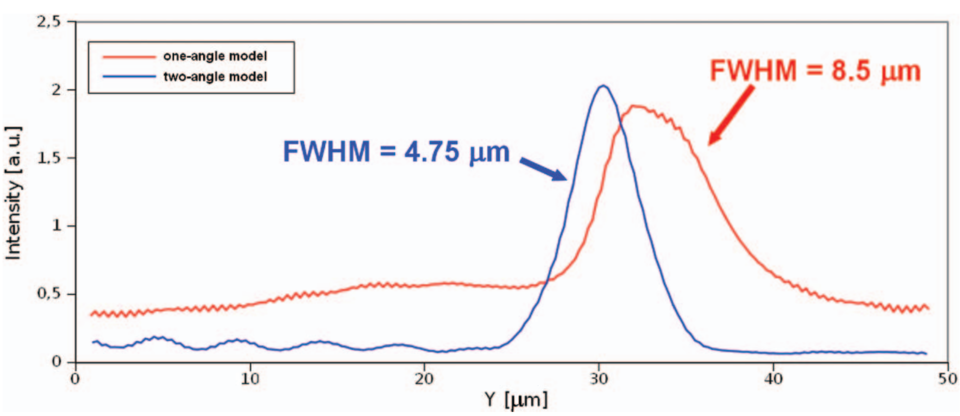

Figure 6. Intensity distribution of the beam cross section at $z = 1000\,\mu$m. The input power P = 60 mW and the beam is polarized at $\alpha = 45^\circ$ and launched $\Delta x = 2\,\mu$m below the center. Graph corresponds to the light intensity distribution in Fig. 5.

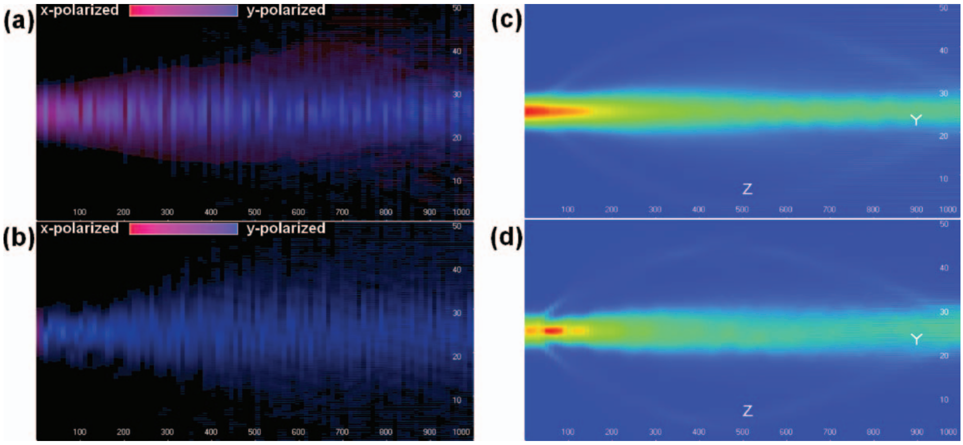

Figure 7. Polarization distribution (left) and light intensity distribution (right) for the input power P = 30 mW and beam polarized at $\alpha = 45^\circ$ launched at the center. Calculations performed using one-angle model (a)(c) and two-angle model (b)(d).

slightly narrower output beam width and shape (see Fig. 8). It is caused by the x-polarized light which in two-angle model destabilizes soliton-like beam. In one-angle model x-polarized light does not affect molecules reorientation so it does not affect soliton-like beam formation.

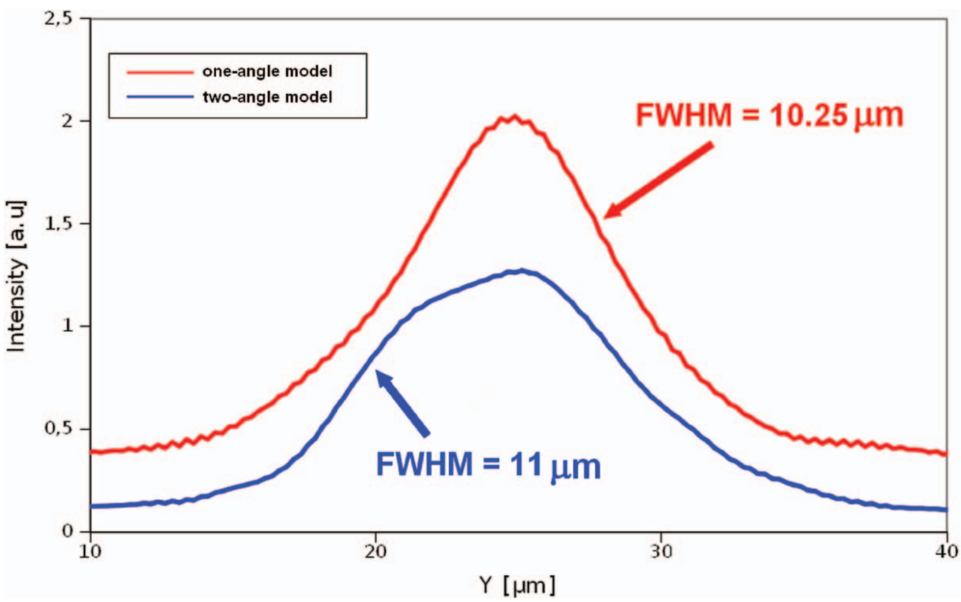

Figure 8. Intensity distribution of the beam cross section at $z = 1000\ \mu$m. The input power P = 30 mW and the beam is polarized at $\alpha = 45^\circ$ and launched at the center. Graph corresponds to the light intensity distribution in Fig. 7.

Conclusions

Full-Vector Beam Propagation Method combined with liquid crystals molecules reorientation model was presented for simulating light propagation in chiral nematic liquid crystals.

Importance of modeling both azimuthal and twist reorientation for particular cases was analyzed. It was presented that simulations using one-angle model result in different polarization distributions and different beam width and shape.

References

[1] Friedel, G. (1922). *Ann. Phys.*, *18*, 273–474.
[2] Oseen, C. W. (1933). *Trans. Faraday Soc.*, *29*, 883–899.
[3] Frank, F. C. (1958). *Discuss. Faraday Soc.*, *25*, 19–28.
[4] Conners, G. H. (1968). *J. Opt. Soc. Am.*, *58*, 875.
[5] Ong, H. L., & Meyer, R. B. (1983). *J. Opt. Soc. Am.*, *73*, 167.
[6] Fleck, J. A. Jr., Morris, J. R., & Feit, M. D. (1976). *Appl. Phys.*, *10*, 129–160.
[7] Ziogos, G. D., & Kriezis, E. E. (2008). *Opt. Quant. Electron*, *40*, 733–748.
[8] Wang, Q., He, S., Yu, F., & Huang, N. (2001). *Opt. Eng.*, *40*, 2552.
[9] Berreman, D. W., & Heffner, W. R. (1980). *Appl. Phys. Lett.*, *37*, 109–111.
[10] Lu, S.-Y., & Chien, L.-C. (2007). *Appl. Phys. Lett.*, *91*, 131119.
[11] Assanto, G., Peccianti, M., & Conti, C. (2003). *Opt. Photon. News*, *14*(2), 44–48.
[12] Laudyn, U. A., Kwasny, M., & Karpierz, M. A. (2009). *Appl. Phys. Lett.*, *94*, 091110.
[13] Laudyn, U. A., Jaworowicz, K., & Karpierz, M. A. (2008). *Mol. Cryst. Liq. Cryst.*, *489*, 214–221.
[14] Assanto, G., & Karpierz, M. A. (2009). *Liq. Cryst.*, *36*, 1161–1172.
[15] Henninot, J. F., Blach, J. F., & Warenghem, M. (2011). *Proc. SPIE*, *8114*, 811406.
[16] Piccardi, A., Alberucci, A., & Assanto, G. (2010). *Appl. Phys. Lett.*, *96*, 061105.
[17] Assanto, G., Skuse, B. D., & Smyth, N. F. (2010). *Phys. Rev. A*, *81*, 063811.
[18] Beeckman, J., Neyts, K., & Haelterman, M. (2006). *J. Opt. A: Pure Appl. Opt.*, *8*, 214.
[19] Assanto, G., & Peccianti, M. (2003). *IEEE J. Quantum Electron.*, *39*, 13.
[20] Skuse, B. D., & Smyth, N. F. (2009). *Phys. Rev. A*, *79*, 063806.
[21] Sala, F. A., & Karpierz, M. A. (2009). *Phot. Lett. Poland*, *1*, 163–165.
[22] de Gennes, P. G., & Prost, J. (1993). *The Physics of Liquid Crystals*, Second Edition, Oxford University Press.
[23] Young, D. M. (1950). *Iterative Methods for Solving Partial Difference Equations of Elliptical Type*, PhD thesis, Harvard University.