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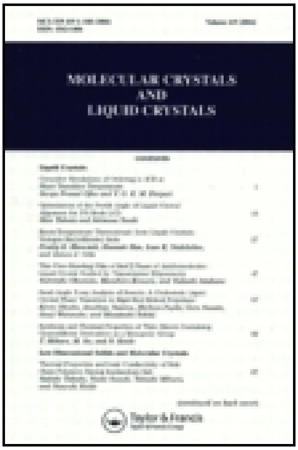

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Simulation of Photorefractive Effect in Thin Liquid Crystal Film

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Simulation of Photorefractive Effect in Thin Liquid Crystal Film

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We study the photorefractive effect in a thin liquid crystal grating by numerical simulation. The cell consists of homeotropically aligned liquid crystal film sandwiched between photo-conductive electrodes. A constant voltage is applied across the cell. The interference pattern from two impinging laser beams then causes a periodic modulation of the potential at the top and bottom surfaces of the liquid crystal cell. We compare results obtained by simulation with an analytical approach which uses the Geometrical Optics Approximation. The results show good agreement between these two methods.

Keywords: finite-difference time-domain method; non-linear optics; photorefractive-like effect

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1. INTRODUCTION

Experimental work in photorefraction in liquid crystals dates back about decade. In the cases of interest in this paper, the effect results

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because a spatially modulated light field causes a modulation of the electric field either in the aligning layer itself [1–5] or in the interface between the LC and the aligning layer [6–8]. In the first case the liquid crystal cell is lined by photoconductive aligning layers, whose electrical resistance is decreased by light irradiation. This increases the electric field in the liquid crystal bulk, which in turn causes a spatially modulated reorientation of the director in the cell. By contrast, in the second case the photorefraction is controlled by the processes in the interface between LC and aligning surfaces. Both of these layers may be nominally insensitive to light. The resultant spatially modulated electric field induces a reorientation of the director in the bulk and a permanent grating.

The key to understanding beam-coupling in these systems lies in the following observation. The surface potential modulation produces a spatially modulated electric field. The resulting torque on the liquid crystal director distorts the initial homogeneous homeotropic alignment. The consequence is an anisotropic medium with a spatially modulated director and hence optical axis. The test beam or the beams that write the grating diffract from the liquid crystal cell, which now possesses a spatially modulated refractive index. One may then calculate beam diffraction and inter-beam energy transfer.

We consider a cell which consists of a homeotropically aligned liquid crystal film sandwiched between photoconductive electrodes. A constant voltage is applied across the cell. The dielectric anisotropy of the liquid crystal material is assumed to be positive. Interference pattern from two impinging laser beams then causes a periodic modulation of the potential at the top and bottom surfaces of the liquid crystal cell. In a related study [9] we have studied the effect of energy exchange in this system phenomenologically. The light propagation through the modulated anisotropic media was treated using the Geometrical Optics Approximation [10–12].

In this paper we study the photorefractive effect in thin liquid crystal grating by numerical simulation. A number of methods are available to study this problem, e.g. the finite-difference method, finite volume, methods of moments, etc. [13]. There are also some approximate methods: Jones matrix 2×2 [14] and Berreman matrix 4×4 [15].

Energy exchange process is a strongly non-linear problem. In principle light propagation should be simulated self-consistently with the director profile calculation. In this work we use a large computational box and simulate the propagation of two plane waves. Another possible approach might involve simulation of one period of the grating with Periodic Boundary Conditions (PBC). However this procedure has not so far been implemented.

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Here we use the director profile analytically calculated in our theoretical paper [9]. We use the FDTD method to solve the Maxwell equations numerically [16]. This method has been widely used in recent years to study complex electromagnetic scattering problems. In particular, the method has been extended to liquid crystals [17–20], and to non-linear liquid crystal optics [21]. This application of the FDTD to the photorefraction problem required a further extension of the numerical algorithm to the case of two incident plane waves. We also compare the results obtained by simulation with an analytical approach using the GOA.

The paper is organized as follows. In §2 we present our model for numerical solution of Maxwell equations with two plane incident waves. In §3 we present results of calculations of energy transfer. The final Section is devoted to a discussion and some conclusions.

2. THEORY

We study the energy exchange effect in the thin liquid crystal film with homeotropic boundary conditions. The liquid crystal cell is sandwiched between photoconductive layers. The geometry of the model is shown on the Figure 1.

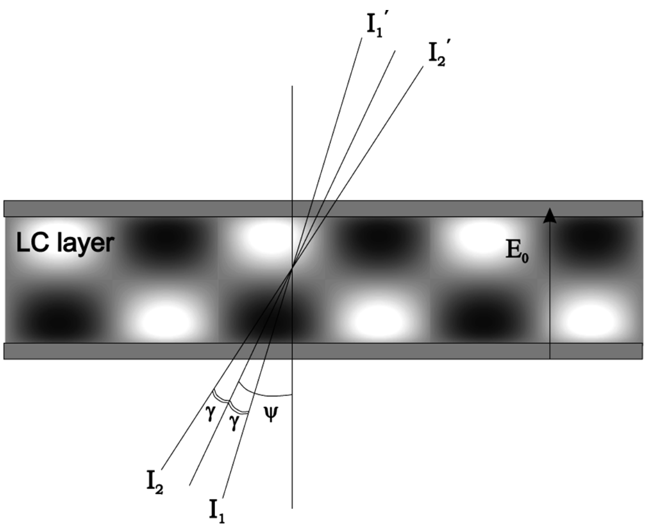

FIGURE 1 Schematic picture of a two-beam coupling experiment, showing meaning of quantities used in the paper.

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TABLE 1 Table of Parameters

Parameter	Value	Description
λ	$0.63\,\mu\text{m}$	Wavelength of incident beams
L	$20\,\mu\text{m}$	Thickness of the film
$\varepsilon_\perp, \varepsilon_\parallel$	1.5^2, 1.7^2	Dielectric permittivities of the liquid crystal
ψ	variable	Angle of propagation inside liquid crystal
δ	$\pi/2$	Phase shift between the interference patterns at top and bottom surfaces. This is the surrogate for the angle of incidence which we do not include explicitly.
q	$k_{1x} - k_{2x}$	grating wave vector
γ	2.4°	Half-angle between beams defining the dimensionless grating wave-vector $\mu = \tilde{q}L = 2kL\sqrt{\frac{\varepsilon_\perp}{\varepsilon_\parallel}}\cos\psi\sin\gamma$
μ	6	Non-dimensional grating wave vector $\mu = \tilde{q}L$. For $\gamma \approx 2.4^\circ, \mu \approx 6$.
ν	1	Dimensionless voltage $\nu = LE_0\left(\frac{\varepsilon_a}{K}\right)^{1/2}$
σ	$\frac{z}{L} - \frac{1}{2}$	Angle of propagation inside liquid crystal
κ	$\sqrt{\mu^2 + \nu^2}$	Model parameter

2.1. The Director Profile

The director profile defines the optical properties of the liquid crystal cell. In our model the interference pattern between incident beams affects the photoconducting layers only by changing the electric potential at the boundaries of the sample. The liquid crystal field is modulated by the periodic modulated potential. Here we use the director deviation $\theta\ (x, z)$ from the perfect homeotropic alignment obtained in our theoretical paper [9].

$$\theta(x,z) = -qL\begin{bmatrix} \cos\frac{\delta}{2}\sin\left(qx + \frac{\delta}{2}\right)\left\{\frac{\cosh\mu\sigma}{\cosh\mu/2} - \frac{\cosh\kappa\sigma}{\cosh\kappa/2}\right\} \\ + \\ \sin\frac{\delta}{2}\cos\left(qx + \frac{\delta}{2}\right)\left\{\frac{\sinh\mu\sigma}{\sinh\mu/2} - \frac{\sinh\kappa\sigma}{\sinh\kappa/2}\right\} \end{bmatrix}. \tag{1}$$

The meaning of the parameters is explained in the Table 1.

2.2. Propagation of Two Plane Waves in Modulated Media

The Maxwell equations in the anisotropic medium are given below, where $\hat{\varepsilon}$ is a tensor susceptibility:

$$\nabla \times \mathbf{E} = -\mu\frac{\partial \mathbf{E}}{\partial t}, \tag{2}$$

$$\nabla \times \mathbf{H} = \frac{\partial}{\partial t}\varepsilon_0\hat{\varepsilon}\mathbf{E}. \tag{3}$$

We solve these equations in time, using the finite-difference time-domain method (FDTD) proposed by Yee [16]. The derivatives in the Maxwell equations change with the finite-differences, taken on the Yee grid for electric and magnetic field. In the Yee grid the electric and magnetic field grids are shifted in the space and time by one half of the grid step. This grid gives an explicit scheme for updating the fields in time. It also automatically satisfies the divergence Maxwell equations. The Yee discretization scheme in the 2D case for the TM_Z (i.e. extraordinary) wave is:

$$E_x\Big|_{i+\frac{1}{2},j}^{n=1} = E_x\Big|_{i+\frac{1}{2},j}^{n} + \Delta t\left[\varepsilon_{xx}^{-1}\Big|_{i+\frac{1}{2},j}\left(\frac{H_z\Big|_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} - H_z\Big|_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta y}\right) - \varepsilon_{xy}^{-1}\Big|_{i+\frac{1}{2},j}\left(\frac{H_z\Big|_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} - H_z\Big|_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta x}\right)\right] \tag{4}$$

$$E_y\Big|_{i,j+\frac{1}{2}}^{n=1} = E_y\Big|_{i,j+\frac{1}{2}}^{n} + \Delta t\left[\varepsilon_{xy}^{-1}\Big|_{i,j+\frac{1}{2}}\left(\frac{H_z\Big|_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} - H_z\Big|_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta y}\right) - \varepsilon_{yy}^{-1}\Big|_{i,j+\frac{1}{2}}\left(\frac{H_z\Big|_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} - H_z\Big|_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta x}\right)\right] \tag{5}$$

$$H_z\Big|_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} = H_z\Big|_{i+\frac{1}{2},j+\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\Delta t}{\mu}\Big|_{i+\frac{1}{2},j+\frac{1}{2}}\left[\frac{E_x\Big|_{i+\frac{1}{2},j+1}^{n} - E_x\Big|_{i+\frac{1}{2},j}^{n}}{\Delta y} - \frac{E_y\Big|_{i+1,j+\frac{1}{2}}^{n} - E_y\Big|_{i,j+\frac{1}{2}}^{n}}{\Delta x}\right] \tag{6}$$

It is a explicit scheme which permits electric and magnetic fields to be calculated in a leapfrog manner. Once E^n is known, fields $H^{n+\frac{1}{2}}$ can be determined from Eq. (6) at all points of the H grid at time step $n+\frac{1}{2}$. At the next time step $n+1$ the E fields can be found from Eqs. (4), (5), and so on.

The plane waves used as the sources of excitation [22]. We extend the FDTD model for the case of two incident plane waves. This allows us to investigate the energy exchange process inside liquid crystal cell directly.

We generate the first plane wave on the virtual boundary between the Total Field and Scatter Field (TF-SF) regions in the computational zone by the Huygens principle [22]. The second plane wave, with a different wave number, is added to the numerical algorithm in the same

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manner as the first plane wave. The field updating scheme is changed only at the TF-SF boundary, where plane waves are generated. We use the perfectly matched layer(PML) [23] as the absorbing boundary conditions to limit the computational zone.

The result of the simulation is the distribution of electric and magnetic fields in the computational zone or near-field zone. However we are interested in the energy exchange between beams. All diffracted orders of the beams can be found in the far-field zone diffraction pattern. Green's theorem is used to determine the projection of electric and magnetic currents from the near-field zone to the far-field zone [22].

3. RESULTS

Firstly, we test the geometric optics approximations used in our previous study [9] of photorefractive-liquid-crystal-induced two-beam coupling against the FDTD solution. The diffraction efficiency for the first order diffracted beam for a thin grating [24] can be obtained from the

$$\eta = J_1^2(2\gamma), \tag{7}$$

where γ is the grating strength parameter given by $\gamma = \frac{\pi\varepsilon_1 d}{2\lambda\sqrt{\varepsilon_0}}$. Here d is thickness of the grating, λ the incident light wavelength, ε_0 is the average dielectric permittivity and ε_1 is the amplitude of the modulation of the dielectric permittivity.

In an ideal case it is either necessary to simulate an infinite grating, or to find a mathematical technique which avoids this necessity. In many apparently analogous cases, the use of Periodic Boundary Conditions (PBC) for the electric and magnetic fields at the computational box boundaries provides such a technique. However, in our case we have two incident plane waves and it is no longer possible to implement PBC consistently. In our work we use a finite box, and investigate the dependence of the calculated η on the number of periods of the grating.

In the numerical experiments we simulate the diffraction of normal incident plane wave from a thin grating. In Figure 2 we show the dependence of η on the size of the grating, measured in terms of the number of grating periods. The results show that for number of periods ≥ 70 the calculated diffraction properties coincide with those calculated theoretically using the GOA.

We have also checked the size of grid step appropriate for our calculations. The dependence of η on the grid step is shown in Figure 3. These results show that the grid step must be $\Delta x \leq \lambda/10$.

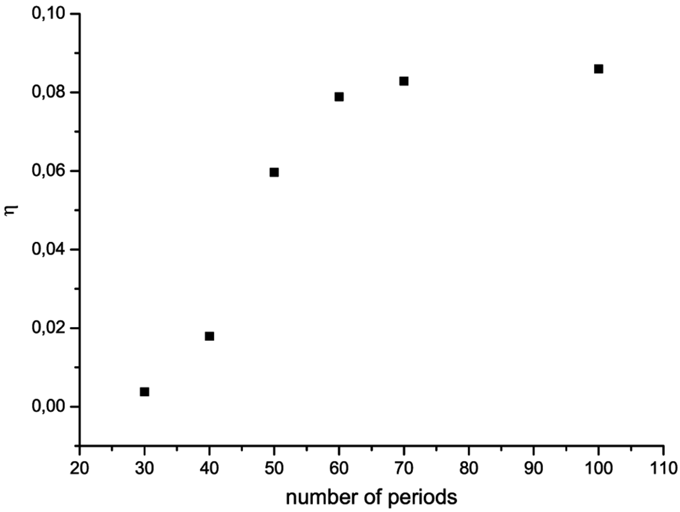

FIGURE 2 The diffraction efficiency for thin grating as a function of number of periods. Grid step is $\Delta x = \lambda/20$. Theoretical value is $\approx$0.082.

In the simulation we measure the beam coupling which is characterized by the *Gain g*. This is the ratio of the intensity of the outgoing beam in the direction of the probe beam I_{12} in the presence of the

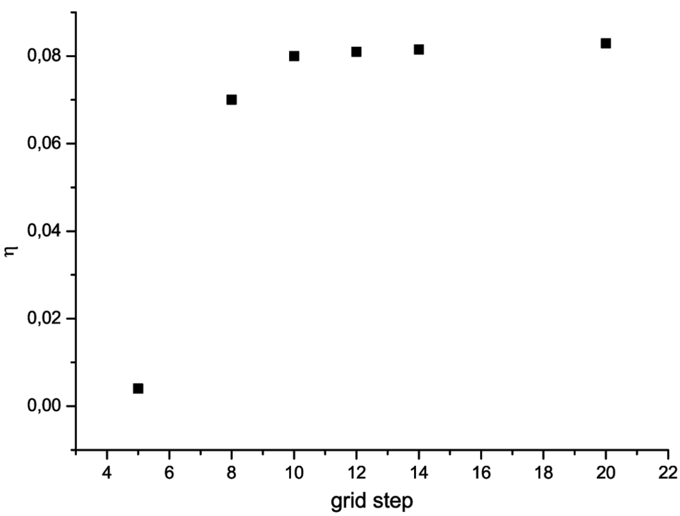

FIGURE 3 The diffraction efficiency for thin grating as a function size of grid step $\Delta x = \lambda$/grid step.

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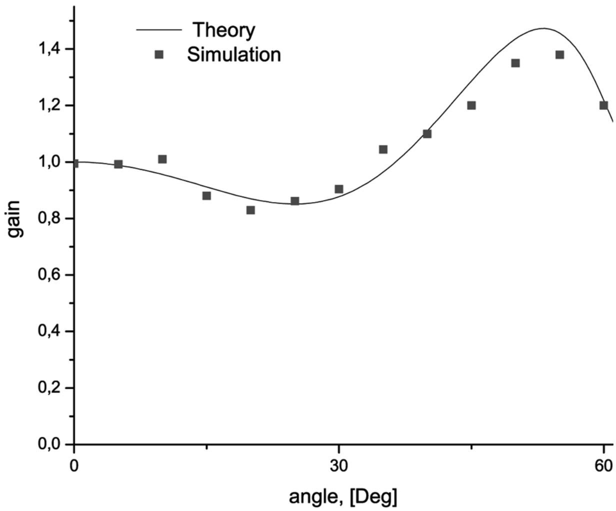

FIGURE 4 Energy exchange between beams as a function of the internal angle ψ.

pump beam to the analogous intensity I_1 in the absence of the pump beam:

$$g = \frac{I_{12}}{I_1}. \tag{8}$$

In order to obtain I_{12} we simulate propagation of two plane waves through the liquid crystal cell with modulated director profile Eq. (1). The quantity I_1 is obtained by simulating the propagation of a single plane wave through the unperturbed liquid crystal cell.

The dependence of the energy exchange as a function of angle of incidence ψ is shown in Figure 4. Our results show good agreement with theory. The deviation of the simulation results from the theoretical curve is of the order of 5%.

4. DISCUSSION AND CONCLUSIONS

This study had a twin set of goals. Firstly, we are testing the geometric optics approximations used in our previous study [9] of photorefractive-liquid-crystal-induced two-beam coupling. Secondly, we are investigating the practicality of using computational optics to study general non-linear beam interactions in liquid crystals.

As far as testing the geometric optics theory [9] is concerned, we need to control other elements of the theory. Thus we use the director

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profile obtained using the elastic theory in [9], even though strictly speaking this also involves some optics. We compare the results of the GOA theory with the exact solution of Maxwell equations. The two-plane wave simulation is used to calculate the optical transmission and hence the energy exchange. The good agreement between the computational and theoretical results in the region where we trust the geometric optics does give ground for optimism that many problems can be solved with our approach. In this paper we present results on the dependence of the energy exchange on the angle of incidence. However the model in principle permits much more extensive investigations.

We have previously found [21] the FDTD method to be useful in modelling the non-linear properties of a single beam. This study involves two beams. We have extended the method to two beams, but the method we have used is so far somewhat computationally awkward. For example, the simulation of the energy exchange is computationally expensive problem. There is as yet no established method of implementing periodic boundary conditions when there is more than one plane wave. We have found that an infinite grating can be approximated by a finite grating whose lateral dimension is more than 70 grating periods. Clearly considerable further benchmarking is required, as well as further investigation of the theoretical basis of the algorithms.

Our method at this stage is relatively primitive, and simply simulates a large system, and waits until convergence has been achieved. At later stage we expect to replace this naive strategy either by an implementation of (quasi-)periodic boundary conditions, or by some more sophisticated finite-size scaling technique. Furthermore, a fully computational technique also requires self-consistent solution of the elastic liquid crystal relaxation, using, for example, a method such as that introduced by Kilian [25].

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