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Finite-difference time-domain calculations of a liquid-crystal-based switchable Bragg grating

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A polymer-wall-confined transmissive switchable liquid crystal grating is proposed and investigated by two-dimensional finite-difference time-domain optical calculation and liquid-crystal-director calculation, to our knowledge for the first time. The results show how to obtain optimized conditions for high diffraction efficiency by adjusting the liquid crystal parameters, grating geometric structure, and applied voltages. The light propagation direction and efficiency can be accurately calculated and visualized concurrently. © 2004 Optical Society of America


1. INTRODUCTION

Switchable liquid crystal gratings play important roles in various optical systems, such as optical interconnects, optical data storage, optical spectral filters, dynamic color rendering for full-color displays, and color-image capture systems. Reference 1 shows three difference approaches to forming the liquid-crystal switchable gratings. The first approach consists of placement of a liquid crystal between two opposing electrodes, at least one of which has been patterned lithographically. Thus when a voltage is applied, a spatially modulated electric field is produced and electro-optically modulates the refractive index of the liquid crystal. A grating is thereby established that will diffract incident light. The advantages of such a device are that it is easy to manufacture and has low-voltage driving. The disadvantages include the slow switching time and the difficulty of forming a thick grating that operates in the Bragg regime. The second approach is a surface-relief pattern filled with liquid crystal and sandwiched between indium-tin-oxide electrodes. Advantages of this device are its manufacturability and low operating voltage. Its disadvantages are low switching speed and low diffraction efficiency. The third approach is a volume hologram, which has been shown to operate in the Bragg regime. One such hologram is a holographic polymer dispersed liquid crystal grating, in which the liquid crystal droplets are formed in periodic layers throughout the sample and are separated by dense polymer layers. This type of grating has been extensively studied.2–5 The advantages of this system are that it yields true Bragg operation with high diffraction efficiency, has a simple single-step fabrication process, and provides fast response speed. Its disadvantage is driving voltage that relatively high compared with that of a bulk liquid crystal device. Coupled-wave theory6 and rigorous coupled-wave analysis7 are commonly used to investigate the diffraction efficiency of a Bragg grating.

In this paper we propose another method to form a switchable liquid crystal grating that is based on a polymer-wall-forming technique. Assuming that both a complete liquid crystal and polymer phase separation occur, then high diffraction efficiency, low-voltage driving, and fast switching speed are expected. Instead of using coupled-wave theory or rigorous coupled-wave analysis, we will accurately analyze the electro-optical characteristics of the device by two-dimensional liquid-crystal-director calculation and finite-difference time-domain (FDTD) optical calculation.

2. DEVICE DESIGN CONSIDERATIONS

The multidimensional alignment method8 can be used to form a periodic polymer wall; the liquid crystal structure and the procedure for forming the polymer wall are shown in Fig. 1. Before UV light exposure, the liquid crystal and the reactive liquid crystal monomers are homogeneously mixed. To obtain low voltage driving, the hybrid liquid-crystal-director configuration is employed. At the cell’s bottom substrate the liquid crystal directors are aligned along the z direction, and at the top they are...
aligned perpendicular to the substrate. During UV light exposure, polymerization-induced phase separation occurs such that polymer walls are formed in UV-exposed areas and the liquid crystal directors are locked in their initial orientation in these walls, which do not respond to the external field. But in the UV non-exposed area, the liquid crystal directors can be reoriented by an external field. Thus a switchable liquid crystal grating is obtained. In order to simplify the liquid-crystal-director calculation, here we assume that the device has complete polymer and liquid crystal phase separation. But in the actual case, one usually cannot obtain this kind of ideal phase separation, which means liquid crystal will exist in the polymer wall and a small amount of reactive liquid crystal monomer will also be left in the liquid crystal region. Especially when the required polymer wall size is small, it is extremely difficult to obtain smooth polymer wall because of diffraction effects, and the driving voltage will increase if polymer cross linking takes place inside the liquid crystal region. In Ref. 8 a qualitative understanding of the multidimensional alignment device is provided that shows how to estimate the distribution polymer inside a liquid crystal pixel with a 100-μm-wide surrounding polymer wall. In our recent fabrication process, we have obtained a smooth 25-μm-wide polymer wall.\textsuperscript{9}
3. CHARACTERIZATION OF THE DEVICE BY COMPUTER SIMULATION

A. Two-Dimensional Liquid-Crystal-Director Calculations

The two-dimensional liquid crystal calculation is based on the LC3D software. The liquid crystal directors at the boundaries, which include top and bottom substrates and surrounding polymer walls, are fixed. Therefore, when the relaxation method is used to calculate the director field, these director orientations at the boundaries will not change. The LC3D program is based on the Frank–Oseen free-energy density given in Eq. (1):

\[
f_g = \frac{1}{2} K_{11} (\nabla \cdot \mathbf{n})^2 + \frac{1}{2} K_{22} (\nabla \times \mathbf{n} + q_0)^2 + \frac{1}{2} K_{33} (\mathbf{n} \times \nabla \times \mathbf{n})^2 - \frac{1}{2} \mathbf{D} \cdot \mathbf{E}.
\]

(1)

Here \( \mathbf{n} \) is the unit vector director; \( K_{11}, K_{22}, K_{33} \) are the liquid-crystal-splay, twist, and bend elastic constants respectively; \( q_0 \) is the chiral wave number (=2 \( \pi / p \) ); \( p \) is the intrinsic chiral pitch of the liquid crystal; \( \mathbf{D} \) is the electric displacement; and \( \mathbf{E} \) is the electric field. The relaxation method is used in our calculation, with the liquid-crystal-director update formula given in Eq. (2), which can be derived from setting the viscous torque equal to the elastic torque:\(^{12}\):

\[
n_i^{\text{new}} = n_i^{\text{old}} - \frac{\Delta t}{\gamma_1} [f_g]_{n_i}, \quad i = x, y, z.
\]

(2)

Here \( \Delta t \) is the numerical time step used in the simulation, \( \gamma_1 \) is the rotational viscosity of the liquid crystal material, \( n_i^{\text{new}} \) denotes the new value of the component of the director, \( n_i^{\text{old}} \) denotes the value at the previous time step, and \([f_g]_{n_i}\) is the functional derivative, given in Eq. (3):

\[
[f_g]_{n_i} = \frac{\partial f_g}{\partial n_i} = \frac{d}{dx} \left[ \frac{\partial f_g}{\partial (dn_i / dx)} \right] = \frac{d}{dy} \left[ \frac{\partial f_g}{\partial (dn_i / dy)} \right].
\]

(3)

In determining the new voltage profile, the direct-solve method removes the requirement of extra iteration. The method is based on the fact that when Gauss’s law (\( \nabla \cdot \mathbf{D} = 0 \)) is discretized, an equation that is linear in the values of the discretized voltage results.\(^{13}\) This equation can then be solved for the new value of the voltage at the current grid point in terms of the values at the surrounding grid points.

The parameters of liquid crystal BL006 (\( ne = 1.816, no = 1.530, \Delta \varepsilon = 10.1 \)) and reactive liquid crystal-monomer RM82 (\( ne \approx 1.656, no \approx 1.532 \)) are used for the liquid-crystal-director calculation. One specific example is considered in following discussion for cell thickness of \( d = 15.0 \mu \text{m} \) and width of liquid crystal and polymer walls 1.0 \( \mu \text{m} \) and 0.5 \( \mu \text{m} \), respectively. The simulated liquid-crystal-director configuration results are shown in Figs. 2(a), 2(c), 2(e), and 2(g), which correspond to applied voltages of 0.0, 5.0, 6.0, and 10.0 V, respectively. Considering the case of incident light polarized along the \( z \) direction, the liquid crystal effective refractive index can be calculated by its director configuration. Figures 2(b), 2(d), 2(f), and 2(h) show the grating device’s effective refractive-index profile at the corresponding voltages of 0.0, 5.0, 6.0, and 10.0 V. Since the boundaries of the polymer wall are assumed to have a strong anchoring condition, the external field will not affect the orientations of the liquid crystal director, and the refractive index is unchanged.

B. Two-Dimensional In-Plane-Grating Equation

In Ref. 14 a general three-dimensional conical diffraction geometry was studied by coupled-wave analysis, and the angle of diffraction for the \( i \)th propagation order was given. For the case of a two-dimensional in-plane grating shown in Fig. 3, the angle of diffraction can be reduced to the well-known grating equation, which is given by Eq. (4):

\[
n_1 \sin \alpha_i + n_3 \sin \beta_m = \frac{m \lambda}{\Lambda_s}, \quad m = 0, \pm 1, \pm 2, \ldots
\]

(4)

\[
\beta_m = \sin^{-1} \left( \frac{m \lambda}{n_3 \Lambda_s} - \frac{n_1}{n_3} \sin \alpha_i \right),
\]

(5)

where \( n_1 \) and \( n_3 \) are the refractive indices of the incident and the exiting media, respectively. Here \( n_1 \) and \( n_3 \) are both in air, so \( n_1 = n_3 = 1.0 \). \( \alpha_i \) is the incident angle of the input light, \( \beta_m \) is the \( m \)th-order diffraction angle of the output light, \( m \) is the diffraction order, \( \lambda \) is the wavelength of the incident light in free space, and \( \Lambda_s \) is the grating periodicity. Equation (5) will be used to verify the diffraction peak position for the FDTD computer simulation results.

C. Finite-Difference Time-Domain Computer Simulation for Light Propagating in the Switchable Liquid Crystal Polymer-Wall Grating

To accurately simulate the light propagating through the switchable liquid crystal polymer-wall grating, a two-dimensional optical calculation is required. Here the FDTD calculation method was implemented.\(^{15-18}\) This method is a numerical approach for directly solving Maxwell’s time-dependent curl equations in a two-dimensional or three-dimensional domain with no other assumptions involved. For sourceless inhomogeneous anisotropic media, Maxwell’s equations can be written as

Fig. 3. Geometrical setup of a two-dimensional in-plane transmissive diffraction grating.
two-dimensional case are given in Eqs. (9) and (10). For the uniaxial liquid crystal case, the electric and magnetic components in Cartesian coordinates and the optical frequencies.

\[
\begin{align*}
\mathbf{E}^{n+1}_z &= \mathbf{E}^n_z + \Delta t \left[ \epsilon_{zz}^{-1} \left( \frac{\partial H^{n+1/2}}{\partial x} - \frac{\partial H^{n+1/2}_y}{\partial y} \right) \right], \\
\mathbf{H}^{n+1/2}_x &= \mathbf{H}^{n-1/2}_x + \frac{\Delta t}{\mu_0} \left( -\frac{\partial E^n_y}{\partial y} \right), \\
\mathbf{H}^{n+1/2}_y &= \mathbf{H}^{n-1/2}_y + \frac{\Delta t}{\mu_0} \left( \frac{\partial E^n_x}{\partial x} \right),
\end{align*}
\]

where \( \Delta t \) is the wave-propagating time step, \( n \) is number of the time step, and \( \epsilon_{zz}^{-1} \) is the zz component in the inverse of the spatially varying dielectric tensor of \( \epsilon(r) \), which here we define as \( \epsilon_{\alpha\beta} \) and \( \alpha, \beta = x, y, z \). The space derivative \( \partial / \partial z \to 0 \), since we consider only two-dimensional calculation in the \( XY \) plane.
For the two-dimensional case (in the XY plane), the near-field to far-field transformation scheme is shown in Fig. 5, and Eq. (12) can be approximated as

\[
\psi_{\text{far}}(x_{\text{far}}, y_{\text{far}}) = \frac{\exp\left((-i \pi)/4\right)}{\sqrt{8 \pi k}} \int_{-d}^{d} \frac{\exp(ikR)}{\sqrt{R}} \left(\frac{\partial}{\partial y}\psi_{\text{near}}(x', y_0)\right) + \frac{i k (y_{\text{far}} - y_0) \psi_{\text{near}}(x', y_0)}{R} \, dx',
\]

where

\[
R = \left[(x' - x_{\text{far}})^2 + (y_0 - y_{\text{far}})^2\right]^{1/2}, \quad k = 2 \pi/\lambda.
\]

Therefore, once near-field two-dimensional FDTD calculation is completed, the far-field diffraction pattern can be calculated by Eq. (13).

The FDTD calculation domain shown in Fig. 4 is illuminated by the z-direction-polarized plane wave from the bottom of the grating with constant amplitude and 30° incident angle with respect to the gratings surface normal. The simulation wavelength in free space is 1.55 μm, and
the optical effects of light propagating through the device


4. CONCLUSIONS

We used the FDTD calculation method to study a new switchable liquid crystal/polymer Bragg grating. The FDTD method exhibits many advantages for characterizing these types of devices: (i) it can accurately calculate the optical effects of light propagating through the device with many different refractive-index profiles without other assumptions; (ii) it can calculate the gratings operated either in the Bragg regime or in the Raman–Nath regime; and (iii) the light propagation can be visualized to aid understanding and to optimize the devices geometric dimensions and the material's physical and optical parameters to achieve high diffraction efficiency. We show that the new switchable Bragg grating has high efficiency and operates at low voltages.

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REFERENCES


