Optimal liquid crystal modulation controlled by surface alignment and anchoring strength

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Spatial modulation of liquid crystals can be controlled and adjusted by light polarization, the degree of pretilt on the substrates, anchoring strength, and the experimental geometry. In particular, strong anchoring can affect the liquid crystal orientation in opposite ways, depending on the polarization of the incident light. Here we present a theoretical model that describes the liquid crystal modulation and how it can be controlled and optimized. The model is valid for electric fields with a uniform component that is large with respect to the spatial modulation, a situation typical of spatial light modulators and photorefractive cells.

1. INTRODUCTION

Liquid crystals are at the heart of many optical devices that are used to modulate, diffract, and, in general, alter the direction, intensity, or polarization of light [1–3]. Two standard examples of such devices in widespread use are spatial light modulators [4–11] and photorefractive cells [12–16]. The common mode of operation of these and other liquid crystal devices is that the voltage applied to the liquid crystal has a uniform component, required to move the liquid crystal past the Fredericks transition, and a generally weaker spatially modulated component that creates a nonuniform director alignment field in the liquid crystal.

The response of a liquid crystal to a given modulated voltage depends on many parameters, from the elastic and dielectric properties of the liquid crystal, to the pretilt and strength of the anchoring at the surfaces. While the role of the former two parameters for reorienting the liquid crystal has been studied in the past [17,18], the importance of the other two parameters (pretilt and anchoring) has not been fully explored.

The influence of different aligning and polymer surfaces on liquid crystal alignment is a topic of increasing interest and importance. This is particularly relevant in the context of liquid crystal based sensors [19]. However, as our model shows, for modulated electric fields integrated in one structure with two polymer surfaces, the effect is equally important. Such consideration is particularly relevant when considering active aligning layers such as photosensitive polymers [14] and liquid crystal metamaterials [20].

As a test structure we consider a typical photorefractive cell that includes a photoconductive alignment layer and a nematic liquid crystal [14], illustrated schematically in Fig. 1. This design was chosen as most appropriate because of its versatility. Such structures are not only used for photorefractive beam coupling, but also form the basis of devices such as spatial light modulators and light valves. However, the theory developed here is not restricted by the details of the device, e.g., the nature of the photoconductive layer, provided that the modeling assumptions are met.

The device consists of a planar cell containing liquid crystals sandwiched between a polyimide (PI) and a photoconducting polyvinyl-carbazole doped with C_{60} (PVK : C_{60}) layer. The superposition of the two coherent incident beams on the photoconductor creates a modulation in the conductivity, which, when combined with the applied DC voltage, produces a modulated electric field across the cell. This aligns the liquid crystals and modulates the refractive index. Such systems have been realized experimentally [13,14] and analyzed theoretically [17,18,21–23]. However, these studies either take a numerical approach to model the liquid crystal alignment [21–23] or consider the case of infinitely strong homeotropic anchoring with simplified forms of the applied electric fields [17,18].

In Section 2, we develop an analytical model of the liquid crystal alignment across the cell based on the following assumptions: (a) the average voltage applied to the cell is sufficiently large to be well past the Fredericks transition; (b) the amplitude of the electric field modulation is small with respect to the average field across the cell; (c) the modulation of the applied voltage varies on a scale comparable with the characteristic length scale of the cell. The first assumption corresponds to the standard working conditions of many liquid crystal devices. The second and third restrict the use of electric fields with too rapid spatial variation. In the photorefractive liquid crystal cell, this effectively acts to restrict the minimum pitch of the grating; however, it is not unduly restrictive. For example, in the case of beam coupling devices, it does not stop the model from being valid in either the Bragg or Raman–Nath regime. We discuss this more in detail in Section 2.

We have checked the accuracy of the model by comparing specific cases with numerical simulations of the director field.

alignment based on the defect free Q-tensor approximation (DFQTA) [22].

In order to understand how the alignment of the liquid crystal affects light propagation, in Section 3 we insert the output of the liquid crystal model into regime independent beam coupling equations [21]. As an example application, this comprehensive model is applied in Section 4 to analyze and understand the diffraction efficiency of a photorefractive cell, like the one in Fig. 1, as a function of cell tilt, anchoring strength, surface pretilt, amplitude of the applied voltage, and polarization of the incoming beams. This analysis reveals some intriguing features of the interactions leading to liquid crystal modulation. One of the most interesting results is that increasing the strength of the anchoring or decreasing the pretilt has the opposite effect on liquid crystal modulation depending on the incident light polarization. Specifically, increasing the anchoring strength or decreasing the pretilt angle has, in general, the effect of increasing the diffraction efficiency of the photorefractive liquid crystal cells. However, if the polarization of the incident light is in the plane of the electric field, then this is seen to decrease the diffraction efficiency. Section 5 concludes the paper with a brief summary and analysis.

2. LIQUID CRYSTAL MODEL

In this section, we develop a model for the alignment of the liquid crystal to a periodically modulated electric field as shown in Fig. 1. We note that although we are interested in a sinusoidal applied potential, we will derive the equations for a much more general class of electric fields. The key assumption that allows us to deal with the modulation is that the strength of the modulated part of the electric field is small relative to the unmodulated part. The cell surfaces are in the x, z-plane with the y-axis normal to the surface. By applying a modulated potential to the cell surface of the form

\[ \psi(x, 0, z) = \psi_0 + \psi_1 \cos(K_y \cdot x), \]  

we obtain a modulated electric field in the cell bulk. Throughout this paper, we will rescale all lengths by the cell thickness \( L_0 \); hence, we obtain the condition \( \psi(x, 1, z) = 0 \) at the far side of the cell. Here the grating vector is restricted to the x, z-plane, \( K_y = K_y \cos \beta \hat{e}_z + \sin \beta \hat{e}_x \), \( K_y = 2\pi L_0 / \Lambda \), and \( \Lambda \) is the grating pitch.

In general, the electric field and the liquid crystal alignment are found by solving a pair of coupled equations. This coupling makes it hard to find analytic solutions. However, for an applied potential with large uniform component, the liquid crystal in the bulk of the cell will be predominantly aligned in the y-direction. Therefore, we approximate the electric potential by solving Maxwell’s equations for a uniform anisotropic medium with optical axis aligned in the y-direction [18],

\[ \epsilon_1 \left[ \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial z^2} \right] + \epsilon_1 \frac{\partial^2 \psi}{\partial y^2} = 0, \]  

(2)

Here \( \epsilon_1 \) and \( \epsilon_0 \) are the components of the dielectric tensor perpendicular and parallel to the liquid crystal director, respectively. This allows us to obtain \( \psi = \psi_0(1 - \rho) + \psi_1 \zeta(x) \), where \( \psi_1 = \frac{K_y \rho}{\psi_0} \ll 1 \),

\[ \zeta(x) = \frac{\sinh [\beta K_y (1 - y)]}{K_y \sinh(\beta K_y)} \cos(K_y \cdot x), \]  

(3)

and \( q = \sqrt{\epsilon_1 / \epsilon_0} \). The corresponding electric field is

\[ E = \psi_0 \hat{e}_y - \psi_1 \nabla \zeta(x). \]  

(4)

For compactness of notation, we define \( \zeta_j(x) = -\hat{e}_j \zeta(x) \) for \( j = \{x, y, z\} \), where

\[ \zeta_x(x) = \frac{\sinh[\beta K_y (1 - y)]}{\sinh(\beta K_y)} \sin(\beta) \sin(K_y \cdot x), \]  

(5a)

\[ \zeta_y(x) = q \frac{\cosh[\beta K_y (1 - y)]}{\sinh(\beta K_y)} \cos(\beta) \sin(K_y \cdot x), \]  

(5b)

and

\[ \zeta_z(x) = \frac{\sinh[\beta K_y (1 - y)]}{\sinh(\beta K_y)} \cos(\beta) \sin(K_y \cdot x). \]  

(5c)

The exact form of \( \zeta \) is not important in the following derivation. The only requirement is that \( |\psi_1 \zeta_j| \ll 1 \) for \( j = \{x, y, z\} \). For \( \psi_1 \sim O(\rho) \), this corresponds to the requirement that \( \zeta \) varies on the same scale as the cell thickness or slower.

We model the orientation of the liquid crystal in terms of a unit director, \( \hat{n} \), which tells us the average alignment of liquid crystal molecules over a small sample. We define \( \hat{n} \) in terms of the first two Euler angles \( \phi \) and \( \theta \). The liquid crystal alignment is found by minimizing the Helmholtz free energy

\[ \mathcal{F} = \int_V \mathcal{F}_d(\hat{n}) + \mathcal{F}_s(\hat{n}) dV + \int_S \mathcal{F}_s(\hat{n}) dS, \]  

(6)

where \( \mathcal{F}_d(\hat{n}), \mathcal{F}_s(\hat{n}), \) and \( \mathcal{F}_s(\hat{n}) \) are the elastic, electrostatic, and surface free energies, respectively. In order to simplify the resulting mathematics, we take the simplest possible forms for these free energies. In nondimensional form, these can be written as

\[ \mathcal{F}_d = \frac{1}{2} |\nabla \theta|^2 + \frac{1}{2} \sin^2 \theta |\nabla \phi|^2, \]  

(7a)
\[ \mathcal{F}_s = -\chi_a [\sin^2 \theta \cos^2 \phi E_x^2 + \sin^2 \theta \sin^2 \phi E_y^2 + \cos^2 \theta E_z^2 \\
+ \sin^2 \theta \cos 2\phi E_x E_y + \sin 2\theta \cos \phi E_y E_z \\
+ \sin 2\theta \sin \phi E_y E_z], \]  
(7b)

and

\[ \mathcal{F}_s = \frac{W_s}{2} [(\phi - \phi_0)^2 + (\theta - \theta_0)^2], \]  
(7c)

where \( \chi_a = \frac{\varepsilon_0 \Delta \varepsilon}{K_d} \psi_0 \), \( W_s = \frac{W_d}{K_d} \), \( E_j = E \cdot \hat{e}_j/\psi_0 \) for \( j = \{x, y, z\} \) are the scaled electric field components, \( \varepsilon_0 \) is the permittivity of free space, \( \Delta \varepsilon \) the dielectric anisotropy of the liquid crystal, \( K_d \) is the elastic constant, \( W_s \) is the surface anchoring strength, and \( \phi_0 \) and \( \theta_0 \) are the preferred orientation of the liquid crystal without loss of generality. Therefore, we describe the liquid crystal by \( \eta \).

We have chosen to use a quadratic form of the surface free energy in Eq. (7c) rather than the more commonly used Rapini–Papoular form of the free energy \([24]\). In general these two forms give the same liquid crystal alignment. The only exception is the limit of very weak anchoring \( W_s \ll O(1) \) in which case Rapini–Papoular saturates to uniform alignment at \( W_s = \sqrt{2} \), whilst the form used in Eq. (7c) saturates to uniform alignment at \( W_s = 0 \). This discrepancy does not change the results qualitatively.

We consider the case where the azimuthal and polar anchoring energies are equal. This assumption is used to simplify the resulting analysis. However, it does not limit the derived equations, which can be applied to the more general case where the azimuthal and polar anchoring energies are different.

The elastic free energy, Eq. (7a), is derived using the one elastic constant limit. Multiple elastic constants can be included in the following derivation but only if the difference between their values can be considered small. We do not expect that including these terms will affect qualitatively the result. They will, however, increase the mathematical complexity of the problem considerably.

In order to understand the effects of the different constants and how they affect the liquid crystal alignment, it is helpful to rescale the free energy. We define the nondimensional variables

\[ \eta = \sqrt{\frac{K_d}{\varepsilon_0 \Delta \varepsilon \psi_0}} \quad \text{and} \quad V_1 = 2K_g \Delta \psi \sqrt{\frac{\varepsilon_0 \Delta \varepsilon}{K_d}} \psi_0 . \]  
(8)

where \( \Delta \psi = \psi_1/\psi_0 \) is defined by the electrical properties of the cell. We also define the scaled anchoring strength \( W_s = \tilde{W_s}/\eta \). Typically we find \( \eta \ll 1 \) and \( V_1 \sim O(1) \). This scaling allows us to neglect terms in the electrostatic free energy of order \( \eta^2 \).

Substituting Eq. (8) into Eq. (7), we derive the Euler–Lagrange equations for the steady state alignment of the liquid crystal. The equation for \( \theta \) is

\[
\nabla^2 \theta - \frac{1}{2} \sin 2\theta |\nabla \phi|^2 \\
+ \frac{1}{\eta^2} \left\{ \sin 2\theta \sin^2 \phi [1 + \eta V_1 \psi_0(x)] \\
+ \eta V_1 \left[ \cos 2\theta \sin \phi \psi_0(x) + \frac{1}{2} \sin 2\theta \cos 2\phi \psi_0(x) \right] \right\} \\
= 0,
\]  
(9a)

the equation for \( \phi \) is

\[
\nabla \cdot (\sin^2 \theta \nabla \phi) + \frac{1}{\eta^2} \left\{ \sin 2\theta \sin^2 \phi [1 + \eta V_1 \psi_0(x)] \\
+ \eta V_1 \left[ -\sin^2 \phi \psi_0(x) + \frac{1}{2} \sin 2\theta \cos 2\phi \psi_0(x) \right] \right\} = 0,
\]  
(9b)

and the boundary conditions are

\[
\frac{\partial \phi}{\partial y} - \frac{\tilde{W_s}}{\eta} (\theta - \theta_0) \bigg|_{y=0} = 0, \quad \frac{\partial \phi}{\partial y} \psi_0(x) \bigg|_{y=0} = 0. \]  
(9c)

To simplify the analysis, we use an infinite anchoring strength condition with zero pretilt at \( y = 1 \). Specifically, this gives us \( \theta(x, 1, z) = \pi/2 \) and \( \phi(x, 1, z) = 0 \).

Equations (9) are a set of nonlinear coupled partial differential equations. In general, these equations do not easily yield an exact analytic solution. Rather, we look for approximate solutions that capture enough of the physics to describe the response of the cell to different anchoring conditions.

To first approximation one approach to solving these equations would be to consider only the terms \( \sim O(1/\eta^2) \). However, this method leaves an algebraic system of equations, the solutions to which will not in general satisfy the boundary conditions at \( y = 0 \) and \( y = 1 \). This type of singular behavior suggests that there must be at least one boundary region close to the cell surface in which the function varies rapidly. Therefore, we look for a solution using the method of matched asymptotics \([25]\).

A. Alignment to a Uniform Field

For a liquid crystal cell described by Eqs. (9), the dominant part of the electric field is the spatially uniform component in the \( y \)-direction. The effect of the modulation is to induce a weak perturbation to this uniform field. Therefore, we first find the alignment of the liquid crystal to the uniform field and then consider how it is perturbed by the modulated part of the electric field.

We write the unknown functions as \( \theta = \theta_0 + \eta \theta_1 + O(\eta^2) \) and \( \phi = \phi_0 + \eta \phi_1 + O(\eta^2) \), where \( \theta_0 \) and \( \theta_1 \) describe the liquid crystal alignment to the uniform field and \( \phi_0 \) and \( \phi_1 \) describe the perturbation of the alignment due to the modulated electric field.

At this point, it is useful to notice that, as we do not restrict the orientation of the grating vector in the \( x, z \)-plane, we are free to choose \( \theta_0 \) without loss of generality. Therefore, we choose \( \theta_0 = \pi/2 \). This ensures that the alignment of the liquid crystal to the uniform field is in the \( x, y \)-plane and that any deviation of \( \theta_0 \) due to the modulated part of the field, is small. The result is that the director can never be aligned along the \( z \)-axis and we do not need to consider the coordinate singularity in the spherical coordinate representation. The uniform alignment equations are found by neglecting the modulated terms in the alignment equations,

\[
\nabla^2 \theta_0 - \frac{1}{2} \sin 2\theta_0 |\nabla \phi_0|^2 + \frac{1}{\eta^2} \sin 2\theta_0 \sin^2 \phi_0 = 0
\]  
(10a)

and
\[ \nabla \cdot (\sin^2 \theta_0 \nabla \phi_0) + \frac{1}{\eta} \sin 2\phi_0 \sin^2 \theta_0 = 0. \]  
\text{(10b)}

We consider three separate regions, the outer region and two inner regions adjacent to the cell boundaries where \( y \sim O(\eta) \) and \( 1 - y \sim O(\eta) \). The unknown functions are denoted \( \theta^{(i)} \) and \( \phi^{(i)} \) in the outer region and \( \theta^{(0)} \) and \( \phi^{(0)} \) in the inner regions.

\[ \sin 2\phi^{(0)} \sin^2 \theta_0^{(0)} = 0, \quad \sin^2 \phi^{(0)} \sin 2\theta_0^{(0)} = 0. \]  
\text{(11)}

Equation (11) has solutions \( \phi^{(0)}_0 = \pi/2 \) or \( \phi^{(0)}_0 = 0 \) and \( \theta_0^{(0)} = \pi/2 \) or \( \theta_0^{(0)} = 0 \). These correspond to the liquid crystal aligned parallel or perpendicular to the electric field. Physically the solution \( \phi^{(0)}_0 = \pi/2 \), corresponding to liquid crystal alignment parallel to the field, is the only stable solution.

The equations in the inner region are found using the substitution \( \bar{y} = y/\eta \) for the region near \( y = 0 \) and \( \bar{y} = (1-y)/\eta \) in the region near \( y = 1 \). For compactness we focus on the inner region near \( y = 0 \). The results obtained can be applied to the region near \( y = 1 \) with minimal effort. However, as the electric field modulation is strongest near the \( y = 0 \) boundary, we expect that there will be little modulation near \( y = 1 \).

As the boundary conditions and electric field restrict the liquid crystal director to the \( x, y \)-plane, we find that \( \theta^{(i)}_0 = \pi/2 \bar{y} \). Physically this corresponds to the liquid crystal director being restricted to the \( x, y \)-plane.

Therefore, we need only consider the equation for \( \phi^{(i)}_0 \). This is the same for both inner regions,

\[ \frac{\partial^2 \phi^{(i)}_0}{\partial y^2} + \sin 2\phi^{(i)}_0 = 0. \]  
\text{(12)}

Integrating once, we obtain

\[ \left( \frac{\partial \phi^{(i)}_0}{\partial y} \right)^2 \cos 2\phi^{(i)}_0 = C_0. \]  
\text{(13)}

The value of the undetermined constant \( C_0 \) is found from the behavior at large \( \bar{y} \). We require that as \( \bar{y} \to \infty \), the behavior of the \( \phi^{(i)}_0 \) tends to that of \( \phi^{(0)}_0 \) \cite{26, 27}. Specifically for large \( \bar{y} \), we require \( \phi^{(i)}_0 = \pi/2 \). Therefore, in order to satisfy Eq. (13), we have \( C_0 = 1 \). Integrating a second time, we find

\[ \phi^{(i)}_0 = -\arctan\left( \frac{C_1 e^{-2\sqrt{2} \bar{y}} - 1}{2C_1 e^{-\sqrt{2} \bar{y}}} \right). \]  
\text{(14)}

The undetermined constant \( C_1 \) is found using the boundary condition at \( \bar{y} = 0 \). Substituting Eq. (13) into (9), we obtain the condition

\[ \frac{\sqrt{2}}{W_s} \cos \phi^{(i)}_0 - (\phi^{(i)}_0 - \phi_s) \bigg|_{y=0} = 0. \]  
\text{(15)}

In general, Eq. (15) must be solved numerically. However, in the limit of strong anchoring \( W_s \gg 1 \), we find \( \phi_0(0) = \phi_s + \sqrt{2}/(2W_s) \cos \phi_s \). Whilst this approximation is derived for large \( W_s \), it is accurate for \( W_s > 1 \). Similarly for \( \bar{W}_s \ll 1 \), we find \( \phi_0(0) = \pi/2 \). In these situations, the undetermined constant can be found using Eq. (14) to obtain

\[ C_1 = \sec \phi^{(i)}_0 - \tan \phi^{(i)}_0 \bigg|_{y=0}. \]  
\text{(16)}

A plot of the director alignment is shown in Fig. 2 for different anchoring strengths and pretilts.

B. Perturbation Due to a Nonuniform Field

Having found the alignment of the liquid crystal to the uniform part of the applied voltage, we now consider how the modulated part of the electric field perturbs the liquid crystal alignment. Substituting \( \theta_0 = \pi/2 \) into Eqs. (9) and retaining terms up to \( O(\eta) \) in the electric field modulation, we obtain

\[ \nabla^2 \phi_1 + \theta_1 \nabla \phi_1 \nabla^2 = \frac{1}{\eta^2} \left[ -2\theta_1 \sin^2 \phi_0 - V_1 \sin \phi_0 \zeta_s(x) \right] = 0 \]  
\text{(17a)}

and

\[ \nabla^2 \phi_1 + \frac{1}{\eta^2} \left[ 2\phi_1 \cos 2\phi_0 + V_1 \sin 2\phi_0 \zeta_s(x) - \cos 2\phi_0 \zeta_s(x) \right] = 0, \]  
\text{(17b)}

with boundary conditions

\[ \frac{\partial \phi_1}{\partial y} - \frac{\bar{W}_s}{\eta} \theta_1 \bigg|_{y=0} \quad \text{and} \quad \frac{\partial \phi_1}{\partial x} - \frac{\bar{W}_s}{\eta} \phi_1 \bigg|_{y=0}. \]  
\text{(17c)}

Again we look for solutions in the inner and outer regions.

In the outer we have

\[ \phi_1^{(i)} = -\frac{V_1}{2} \zeta_s(x) \quad \text{and} \quad \phi_1^{(i)} = \frac{V_1}{2} \zeta_s(x). \]  
\text{(18)}

![Fig. 2. (Color online) Plots of \( \phi_0 \) as a function of the distance into the cell for different values of the anchoring energy (top) and of the pretilt angle at \( y = 0 \) (bottom).](image-url)
Therefore, as \( \zeta_z \) and \( \zeta_x \) have sine-like modulation, for all \( \beta \) there is a grating in the outer region that is out of phase by \( \pi / 2 \) with the voltage modulation.

The inner equations are obtained by rescaling Eqs. (17) as in the uniform electric field case, \( \tilde{y} = y/\eta \) for the region near \( y = 0 \) and \( \tilde{y} = (1 - y)/\eta \) in the region near \( y = 1 \). Substituting \( \theta^{(i)}_0 \) into Eqs. (17), we obtain

\[
\frac{\partial^2 \theta^{(i)}_1}{\partial \tilde{y}^2} + 2 \theta^{(i)}_0 \cos 2\phi^{(i)}_0 = F_{\theta}(\phi^{(i)}_0),
\]

\[
\frac{\partial^2 \phi^{(i)}_1}{\partial \tilde{y}^2} + 2 \phi^{(i)}_0 \cos 2\phi^{(i)}_0 = F_{\phi}(\phi^{(i)}_0),
\]

where the source terms are

\[
F_{\theta}(\phi^{(i)}_0) = \sin \phi^{(i)}_0 V_1 \zeta_z(x),
\]

\[
F_{\phi}(\phi^{(i)}_0) = V_1 (\cos 2\phi^{(i)}_0 \zeta_x(x) - \sin 2\phi^{(i)}_0 \zeta_y(x)).
\]

(20)

The key observation that allows a solution to be obtained is that \( \zeta \) varies on a scale \( \sim O(\eta^2) \) and may be treated as a constant in the inner region. As in the uniform case, we only present solutions near \( y = 0 \), as this is where the majority of the modulation occurs. The resulting equations can easily be applied to the boundary near \( y = 1 \) with minimal modification.

Substituting Eq. (14) into Eqs. (19) and using \( \theta^{(i)}_1 \rightarrow \theta^{(i)}_0 \) and \( \phi^{(i)}_1 \rightarrow \phi^{(i)}_0 \) as \( \tilde{y} \rightarrow \infty \), we find

\[
\theta^{(i)}_0 = \frac{V_1}{2} \left[ 1 - e^{\sqrt{2}y} + e^{\sqrt{2}y} \right] \zeta_z(x),
\]

(21a)

\[
\phi^{(i)}_0 = \frac{V_1}{2} \left[ C_1 \left( e^{\sqrt{2}y} + 2e^{\sqrt{2}y} \right) \right] \zeta_x(x).
\]

(21b)

To find the undetermined coefficients, we use the boundary conditions (17c):

\[
C_\phi = -\frac{C_1[(1 + C_1^2)\tilde{W}_s - \sqrt{2}(1 + 3C_1^2)]}{(1 + C_1^2)\tilde{W}_s + \sqrt{2}(1 - C_1^2)}.  
\]

(22)

\[
C_\phi = \frac{(C_1^2 + 1)\tilde{W}_s}{(-W_s - W_s C_1^2 - \sqrt{2} + \sqrt{2}C_1^2)}.  
\]

(23)

and

\[
C_\theta = \frac{(C_1^2 + 1)\tilde{W}_s + 4\sqrt{2}C_1^2}{(C_1^2 + 1)W_s - \sqrt{2}(C_1^2 - 1)}.  
\]

(24)

The composite expansion is obtained by adding the inner and outer solutions at each order and subtracting the common parts. In this case, such a matching is trivial as the outer solution is the common part. Therefore, if we denote the inner solution near \( y = 0 \) as \( \theta_p^{(i,j)} \), \( \phi_p^{(i,j)} \), and the inner solution near \( y = 1 \) as \( \theta_p^{(i,j)} \), \( \phi_p^{(i,j)} \), where \( p = 0,1 \) denotes the order of the terms; the composite expansion, neglecting terms \( \sim O(\eta^2) \), is

\[
\theta = (\theta_0^{(i,j)} + \theta_p^{(i,j)} - \theta_0^{(i,j)}) + \eta(\theta_1^{(i,j)} + \theta_p^{(i,j)} - \theta_0^{(i,j)})
\]

\[
\phi = (\phi_0^{(i,j)} + \phi_p^{(i,j)} - \phi_0^{(i,j)}) + \eta(\phi_1^{(i,j)} + \phi_p^{(i,j)} - \phi_0^{(i,j)}).
\]

(25)

These equations provide an approximate description of how the liquid crystal aligns to large electric fields. The alignment to the uniform field, \( \theta_0 \) and \( \phi_0 \), can be considered exact for any voltages that are large enough to fully align the liquid crystal in the center of the cell such that \( \theta_0(1/2) = \phi_0(1/2) = \pi/2 \).

The alignment of the liquid crystal to the modulated field uses the approximation \( V_1 \sim O(1) \). However, the model can still provide a reasonably accurate description for \( V_1 \lesssim O(1/\eta) \).

3. OPTICAL MODEL

The coupling of optical beams via the liquid crystal grating relates to the optical dielectric tensor. This has the form

\[
e = e_u + \Delta e Q,\]

where

\[
e_u = \frac{e_u + 2e_\perp}{3} \quad \text{and} \quad \Delta e = e_\parallel - e_\perp.
\]

(26)

The nonhomogeneous part of the dielectric tensor is given by

\[
Q = \hat{n} \otimes \hat{n} - 1/3I \quad [28].
\]

To order \( \eta \), we can write

\[
Q = Q_u + \eta(Q_{\phi\theta} \phi_1 + Q_{\theta\phi} \theta_1).
\]

(27)

where, for \( \theta_0 = \pi/2 \),

\[
Q_u = \frac{1}{2} \begin{pmatrix}
(1 + \cos 2\theta_0) & -\frac{1}{3} & \sin 2\theta_0 \\
\sin 2\theta_0 & 1 - \cos 2\theta_0 & 0 \\
0 & 0 & 1
\end{pmatrix},
\]

(28)

and the modulation coefficients for \( \theta_1 \) and \( \phi_1 \) are given by

\[
Q_{\phi} = \begin{pmatrix}
-\sin 2\theta_0 & \cos 2\theta_0 & 0 \\
\cos 2\theta_0 & \sin 2\theta_0 & 0 \\
0 & 0 & 0
\end{pmatrix},
\]

(29)

and

\[
Q_{\theta} = \begin{pmatrix}
0 & 0 & -\cos \phi_0 \\
0 & 0 & -\sin \phi_0 \\
-\cos \phi_0 & -\sin \phi_0 & 0
\end{pmatrix}.
\]

To study the diffraction of a beam incident on the photorefractive cell, we make use of the regime independent beam coupling model [21]. The coupled wave equations are derived by considering the nonhomogeneous parts of the dielectric tensor as a perturbation for small optical anisotropy.

The key parameter that determines the diffraction efficiency is the coupling coefficient:

\[
\kappa_{n,n+1} = \hat{E}(n) : [Q_{\phi}(\phi_{1,c} + i\phi_{1,s}) + iQ_{\theta}(\theta_{1,s})] \hat{E}^{*(n+1)},
\]

(30)

where \( \hat{E}(n) \) is the normalized electric field polarization of the \( n \)-th wave and for compactness of notation we have defined
\( \phi_1 = \phi_{1,e} \sin K_y \cdot x + \phi_{1,c} \cos K_y \cdot x \) and \( \theta_1 = \theta_{1,e} \sin K_y \cdot x \).

The modulation of \( \theta_1 \) is of the form \( \sin K_y \cdot x \forall \beta \). This is out of phase by \( \pi/2 \) with the applied voltage. The modulation of \( \phi_1 \) has components that are both sine and cosine like (see Eq. (21b)), and moves from being in phase with the applied voltage for \( \beta = 0 \) to having components both in phase and out of phase by \( \pi/2 \) for \( \beta = \pi/2 \). The relative phase of the sine and cosine like terms only comes into play for beam coupling experiments where the net energy transferred between beams is a superposition of the two different diffracted beams.

To analyze the effects of the modulation of the optical field, it is convenient to introduce the component representation of the \( Q \)-tensor [29],

\[
Q = \sum_{\nu=1}^{5} a_{\nu} T^{(\nu)},
\]

(31)

where

\[
T^{(1)} = [\hat{\mathbf{e}}_x \otimes \hat{\mathbf{e}}_x - \hat{\mathbf{e}}_y \otimes \hat{\mathbf{e}}_y + 2 \hat{\mathbf{e}}_z \otimes \hat{\mathbf{e}}_z],
\]

\[
T^{(2)} = [\hat{\mathbf{e}}_x \otimes \hat{\mathbf{e}}_x - \hat{\mathbf{e}}_y \otimes \hat{\mathbf{e}}_y],
\]

\[
T^{(3)} = [\hat{\mathbf{e}}_x \otimes \hat{\mathbf{e}}_y + \hat{\mathbf{e}}_y \otimes \hat{\mathbf{e}}_x],
\]

\[
T^{(4)} = [\hat{\mathbf{e}}_x \otimes \hat{\mathbf{e}}_z + \hat{\mathbf{e}}_z \otimes \hat{\mathbf{e}}_x],
\]

\[
T^{(5)} = [\hat{\mathbf{e}}_y \otimes \hat{\mathbf{e}}_z + \hat{\mathbf{e}}_z \otimes \hat{\mathbf{e}}_y].
\]

(32)

Verification of the liquid crystal model is achieved through numerical comparison to the DFQTA [22]. As a measure of the error we use

\[
e_r = \frac{||a_1 - a_{\text{num}}||}{||a_1||},
\]

(33)

where \( a_{\text{num}} \) is the numerically determined Fourier coefficient of the fundamental component of the modulation for an electric field as given in Eq. (4), and \( a_1 \) is the approximate representation of the first order correction as derived here. This measure is chosen as it reflects the error in the diffraction induced by the fundamental grating vector. It should be noted that this measure neglects the higher harmonics of the grating vectors induced by the quadratic terms in the electric field. However, in general, these will be comparable with \( e_r \) and will not provide a strong contribution to the diffraction. The calculated error is small in all cases of interest with \( e_r = 0.016 \) for \( \psi_0 = 30 \text{ V} \) and \( \delta \psi = 0.01 \) and \( e_r = 0.038 \) for \( \psi_0 = 10 \text{ V} \) and \( \delta \psi = 0.05 \).

The relative amplitude and phase of the different components are shown in Figs. 3 and 4 for \( \psi_0 = 5 \text{ V} \) and \( \delta \psi = 0.05 \). We note that for these values of \( \psi_0 \) and \( \delta \psi \), the error is relatively large \( e_r \approx 0.072 \). However, these figures do provide a clear image of how the liquid crystal aligns in the whole cell and in which regions the modulation is strongest. Using a higher voltage, for which the error would be lower, causes the inner region to become very thin and, hence, makes the features harder to observe. The components and how they affect the diffraction efficiency will be discussed in Section 4.

4. ANALYSIS OF RESULTS

We now want to apply the model developed in the previous section to study the effect of pretilt, anchoring strength, and cell tilt on the cell diffraction efficiency and, hence, the beam coupling strength. Before doing this, we recall the range of validity of the model: we assume that the voltage applied to the cell is sufficiently large to be past the Fredericks transition and that the modulated component of the electric field is small with respect to the average field across the cell. As discussed in the previous section, these constraints are not unduly restrictive and, in fact, the results discussed in this section apply to most standard configurations of beam coupling devices.

Using the parameters given in Table 1, we consider three cases: transverse electric (TE), transverse magnetic (TM), and in-plane polarization as defined in Fig. 5. We discuss the diffraction efficiency for these three configurations in detail in the next three subsections. Rather than study beam coupling separately, we use the fact that the beam coupling in these cells is surface mediated. Therefore, the coupled intensity of two incident beams is simply a superposition of the amplitudes of the first diffracted order of each beam and the zeroth order of the other. We can consider the diffraction efficiency as an upper bound on the strength of coupling between the two beams.

A. Transverse Electric Polarization

In the TE configuration, the incoming light beam has an electric field linearly polarized in the \( x \)-direction (see Fig. 5) and parallel to the surface alignment of the liquid crystal.

The anisotropic diffraction grating in the liquid crystal acts not only to couple light into different directions but also into waves with different polarizations. To understand these effects, we break Eq. (30) into three different components:

\[
\kappa^{(E,E)}_{n,n+1} = c_x^{(n)} a_2 c_x^{(n+1)},
\]

(34a)

\[
\kappa^{(E,M)}_{n,n+1} = d_3 \left( c_x^{(n)} c_y^{(n+1)} + c_y^{(n)} c_x^{(n+1)} \right)
\]

\[
+ d_4 \left( c_x^{(n)} c_z^{(n+1)} + c_z^{(n)} c_x^{(n+1)} \right),
\]

(34b)

\[
\kappa^{(M,M)}_{n,n+1} = d_5 \left( c_y^{(n)} a_2 c_y^{(n+1)} + a_5 \left( c_y^{(n)} c_z^{(n+1)} + c_z^{(n)} c_y^{(n+1)} \right) \right),
\]

(34c)

and \( \kappa^{(E,M)}_{n,n+1} = \left( \kappa^{(E,M)}_{n,n+1} \right)^* \), where * denotes complex conjugate and \( c_j^{(n)} = \hat{e}_j \cdot \hat{e}_j^{(n)} \) for \( j = \{ x, y, z \} \). Equation (34a) describes the coupling from TE to TE polarized waves, Eq. (34b) describes the coupling from TE to TM and TM to TE polarized waves, and Eq. (34c) describes the coupling from TM to TM polarized waves.

We consider first the case of zero cell tilt (normal incidence). The field at input has zero \( y \)- and \( z \)-components. Propagation in the liquid crystal will couple this field with other TE modes through Eq. (34a), but also to TM modes through Eq. (34b). These will have both a \( y \) and a \( z \)-component, but the former is much smaller than the latter. Therefore, we can conclude that the coupling in this system is determined mainly by the coefficients \( a_2 \) and \( a_5 \) of the \( Q \)-tensor field. These are relatively small and concentrated near the boundary (see Fig. 3);
therefore, we expect that the diffraction efficiency will be relatively small. Decreasing the anchoring energy, increasing the pretilt angle or the voltage applied to the cell reduces the range where the modulation of the liquid crystal can be effective: in the limiting case of a pretilt angle $\phi_a = \pi/2$ or very weak anchoring energy or strong field, the alignment is homeotropic across the cell and the only modulation possible is in the $(y, z)$-plane, to which an $x$-polarized field is insensitive. We therefore expect that the diffraction efficiency will decrease in all these cases. These considerations are borne out by the results of the beam coupling model (34). In the top two panels of Fig. 6, we plot the logarithm of the amplitude of the $-1$ diffracted order as a function of the pretilt angle at infinite anchoring energy at zero pretilt angle (right). The scale of the figure indicates that the diffraction efficiency is small (max. value $\sim 1\%$); moreover, its general trend is to decrease with increasing pretilt angle or voltage and decreasing anchoring energy, even though the decrease with the latter is not monotonic.

A look at Fig. 5 shows that a nonzero cell tilt does not change qualitatively the physics of the system. In fact, if the cell tilt is different from zero, the $y$- and $z$-components of the excited TM modes are comparable in size. Therefore, the coupling also involves the $a_3$ coefficient. This has very similar behavior to $a_2$ and $a_4$ (see Fig. 3). Hence, we expect that the diffraction efficiency will be similar to the normal incidence case. This is confirmed by the bottom two panels of Fig. 6, which are very similar to the top two.

B. Transverse Magnetic Polarization

In the TM configuration, the incoming light beam has an electric field linearly polarized in the $(y, z)$-plane, is orthogonal to the surface alignment of the liquid crystal, and forms an angle with the $x$-axis equal to the cell tilt (see Fig. 5).

We consider first the case of zero cell tilt (normal incidence). The field at input has zero $x$- and $y$-components. The modulation of the liquid crystal out of the $(x, y)$-plane induces orders with nonzero $x$- and $y$-components; in particular, it can couple the $z$-component of the TM input field with the (very small) $y$-component of another TM mode through Eq. (34c), but, much more importantly, also to the (order one) $x$-component of a TE mode through Eq. (34b). Therefore, the diffraction efficiency is dominated by the $a_4$ coefficient of the $Q$-tensor field. We can see from Fig. 3 that this decreases monotonically to zero with the pretilt angle and asymptotically, but not monotonically, with the anchoring energy. Increasing the voltage at fixed modulation amplitude reduces the thickness of the boundary layers at $y = 0$ and $y = 1$ and, hence, the regions where $a_2$ and $a_4$ are different from zero. Therefore, we expect that the diffraction efficiency decreases with increasing $\psi_0$. All these considerations are borne out by the results of the beam coupling model (34), presented
in the top two panels of Fig. 7. The scale of the figure indicates that the diffraction efficiency is smaller (max. value \( \sim 0.1\% \)) than in the TE case and that its general trend is to decrease with increasing pretilt angle and decreasing anchoring energy. Note that the nonmonotonic behavior of the diffraction efficiency with fixed pretilt is more pronounced in this case than in the TE configuration.

If the cell tilt angle is different from zero, then the input field and the first diffracted orders have nonzero components in both the \( y \)- and \( z \)-directions. In this case, the coupling between orders is caused mainly by the rather large \( a_5 \)-component of the director field, as can be seen in Eq. (34c). Not only is this component relatively large, but it extends quite considerably in the cell (see Fig. 3). Moreover, it is relatively independent of the pretilt angle and of the anchoring energy. Therefore, we expect that the diffraction efficiency in this configuration will be relatively large and uniform. This is confirmed by the bottom two panels of Fig. 7, which have a very limited range of values.

C. In-Plane Polarization

In the in-plane configuration, the incoming light beam has an electric field linearly polarized in the \((x, y)\)-plane and forms an angle with the \( x \)-axis equal to the cell tilt (see Fig. 5).

In this configuration, the liquid crystal modulation is restricted to the \((x, y)\)-plane. Therefore, Eq. (30) can be written as

\[
\kappa_{n,m=\pm 1}^{(P, P)} = a_2 \left( \varepsilon_x^{(n)} \varepsilon_x^{(n+1)} + \varepsilon_y^{(n)} \varepsilon_y^{(n+1)} \right) + a_3 \left( \varepsilon_x^{(n)} \varepsilon_y^{(n+1)} + \varepsilon_y^{(n)} \varepsilon_x^{(n+1)} \right),
\]
where, in this case, $a_2$ and $a_3$ have both sine and cosine like modulation. In the bulk of the cell the TM and in-plane configurations are the same, but they differ in the relative orientation of the light polarization and director field near the surfaces. We expect, therefore, that the diffraction efficiency of the two configurations should be comparable, which is indeed the case.

We consider first the case of zero cell tilt (normal incidence). The field at input has zero $y$- and $z$-components. The modulation of the liquid crystal induces orders with nonzero $y$-components, but still very small in comparison with their corresponding $x$-components. By looking at Eq. (35),

we see that the only significant coupling is through the $a_2$-component of the $Q$-tensor. From Fig. 4, we see that this component is not large; it decreases with increasing pretilt angle and also goes asymptotically (but not monotonically) to zero with weakening anchoring energy. As usual, increasing the voltage shrinks the boundary layers and makes the diffraction efficiency smaller. These observations are confirmed by the top two panels of Fig. 8: the in-plane configuration at normal incidence is in all respects very similar to the corresponding TM configuration.

If the cell tilt angle is different from zero, then the input field and the first diffracted orders have nonzero components in both the $x$- and $y$-directions. In this case, even though all components of the $Q$-tensor contribute to the coupling, the sine-like component of the $a_2$ coefficient plays a key role, because of its magnitude, especially for large pretilt and weak anchoring, and the fact that it is nonzero across the cell (see Fig. 4). This component is relatively independent of the pretilt angle and of the anchoring energy. Therefore, we expect that the diffraction efficiency in this configuration will be relatively large and uniform. This is confirmed by the bottom two panels of Fig. 8, which have a limited range of values (though larger than the corresponding TM configuration).

5. CONCLUSION

In this paper, we have derived and analyzed a model for the alignment and optical response of liquid crystals subject to different surface alignments and cell geometries. The liquid crystal is aligned by a uniform field that is large enough to align the liquid crystal in the center of the cell. The liquid crystal alignment is then perturbed by a relatively small modulated part, which varies with the characteristic length scale of the geometry, in this case the cell thickness.

To model the optical response, we have used coupled wave theory [21]. This allows us to calculate the diffraction efficiency of the cells subject to the different control parameters. We have studied three different cases in detail and have found

Fig. 6. (Color online) Contour plots of the first order diffraction efficiency in the TE configuration as a function of the applied voltage and (left) the pretilt at anchoring energy $W_s = 10^8$ or (right) the logarithm of the anchoring energy at zero pretilt angle for 0 (top) and 35° cell tilt (bottom). The color coding is logarithmic base 10, with −1 corresponding to 10% of the input power being transferred from the input beam to the −1 diffracted order.

Fig. 7. (Color online) Same as Fig. 6, but for the TM configuration.

Fig. 8. (Color online) Same as Fig. 6 but for the in-plane configuration.
that, as a general trend, the diffraction efficiency of the optical beams is decreased with decreasing anchoring strength or increasing pretilt. There are two exceptions when this is not the case. These are the in-plane and TM cases with 35° cell tilt. In these cases the coupling is dominated by the modulation of the electric field in the cell bulk rather than in the boundary layers. Decreasing the anchoring strength or increasing the pretilt in these areas increases the length of the interaction region and, hence, increases the diffraction efficiency.

The strongest diffraction efficiency is obtained for beams that are polarized in the plane formed by \( K_\parallel \) and the \( y \)-axis with nonzero cell tilt. In these cases it is desirable to have homeotropic or weak anchoring conditions in order to maximize the diffraction efficiency.

In obtaining these results, we have used the one elastic constant approximation to simplify the elastic free energy. Multiple elastic constants could be included as a perturbation. The analysis could also be extended, without altering the derivation, for the case where the polar and azimuthal anchoring strengths are different. One interesting extension of this work would be to include flexoelectric terms in the bulk and surface free energies allowing the work presented here to be applicable to a larger group of liquid crystals.

The results presented in this paper highlight the importance of optimizing a whole set of material and device parameters to achieve strong modulation rather than, for example, a single property of the liquid crystal such as birefringence. The knowledge and control of anchoring and pretilt is essential to ensure the strongest possible optical response of liquid crystals. The model described here makes it possible to determine the contribution from different liquid crystal and structure parameters and to simulate the performance of devices with different electric fields. Therefore, it should prove useful as a tool in optimization of liquid crystal modulators and cells.

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