2D director calculation for liquid crystal optical phased array

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Abstract. A practical numerical model for a liquid crystal cell is set up based on the geometrical structure of liquid crystal optical phased arrays. Model parameters include width and space of electrodes, thickness of liquid crystal layer, alignment layers and glass substrates, pre-tilted angles, dielectric constants, elastic constants and so on. According to electrostatic field theory and Frank-Oseen elastic continuum theory, 2D electric potential distribution and 2D director distribution are calculated by means of the finite difference method on non-uniform grids. The influence of cell sizes on director distribution is analyzed. The fringe field effect between electrodes is also discussed.

1. Introduction
Optical phased arrays (OPA) can be implemented using liquid crystals to produce the phase shift. Liquid crystal modulators offer several advantages including large modulation depth, inertialess switching, low power dissipation, low cost, and random-access beam steering [1]. In the design of liquid crystal optical phased arrays (LCOPA), we need to consider the sizes of liquid crystal cell and analyze its influence on device performances. Therefore, it is necessary to set up a suitable numerical model for a liquid crystal cell. The director calculation is critical because it determines the relationship between driving voltage and corresponding phase delay, and it is also the theoretical base for LCOPA to accomplish non-mechanism electro-controlled beam steering.

Recently, most approaches to calculate liquid crystal director have been based upon Frank-Oseen elastic continuum theory. These approaches include Newton’s method, relaxation method, finite difference iterative method and simulated anneal method [2]. Calculation techniques in relaxation method include finite element method [3] and finite difference method [4], and we adopt the latter.

In this paper a practical model is set up based upon the geometry structure of LCOPA. And finite difference method is used to calculate 2D director distribution. Because the iterative algorithm is used, it is necessary to provide initial values of director and potential to start up iterative. Here, we give the accurate initial values by calculation. The fringe field effect in LCOPA is also discussed.

2. Numerical model
Typical structure of liquid crystal cell consists of several layers: upper glass substrate, upper and lower ITO electrodes, upper and lower alignment layers and liquid crystal layer. The liquid crystal cell’s model is set up, as is illustrated in Figure 1.
Figure 1. The numerical model of liquid crystal cell. Physical parameters we used are:

\[ K_{11} = 11.1 \times 10^{-12} \text{N}, \quad K_{33} = 17.1 \times 10^{-12} \text{N}, \]
\[ \varepsilon_{\parallel} = 19.0, \quad \varepsilon_{\perp} = 5.2, \quad \varepsilon_{\text{glass}} = 3.5, \quad \varepsilon_{\text{film}} = 3.0. \]

Two pre-tilted angles are 2° and 5°, respectively.

3. Numerical calculation

3.1. Frank-Oseen theory

The vector approach [5] is employed to represent the director: \( \mathbf{n} = (n_x, 0, n_z) \). According to Frank-Oseen theory, the Gibbs free energy density in liquid crystal cell is expressed as following:

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

Where \( K_{11}, K_{22}, K_{33} \) are the splay, twist and bend constants, respectively; \( \mathbf{D} = \varepsilon \mathbf{E}, \mathbf{E} = -\nabla \varphi \) are electric displacement and electric field intensity, respectively. Where \( \varphi \) is potential and \( \varepsilon \) is dielectric tensor of liquid crystal material, \( \varepsilon_{\parallel} = \varepsilon_{\perp} \delta_{ij}^\parallel + \Delta \varepsilon n_j, \Delta \varepsilon = \varepsilon_{\parallel} - \varepsilon_{\perp} \).

3.2. Director calculation method

The idea to calculate 2D director is that: the Gibbs free energy will attain its minimum when the liquid crystal molecules are in equilibrium. Calculate the variation of Gibbs free energy density and let the variation equals to zero, then the Euler-Lagrange equations with regard to director \( \mathbf{n} \) and potential \( \varphi \) are derived as below:

\[
0 = -[f_G]_{\mathbf{n}} = \nabla \cdot (\mu_i \nabla \varphi)
\]
\[
0 = -[f_G]_{\varphi} + \lambda n_i, i \in (x, y, z)
\]

Where \( \lambda \) is Lagrange multiplier used to maintain \( \mathbf{n} = 1 \). We calculate the Euler-Lagrange equations by means of finite difference method on non-uniform grids.

3.3. Initial Director Calculation
Director calculation is an iterative process and needs suitable initial values to start up. Initial values are important as they affect convergence speed and reliability of iteration. In fact, the accurate initial values of director and potential can be obtained by calculation.

Initial director can be given by 1D simulation [6]. To equation (1), let the item \(-\frac{1}{2}(\vec{D} \cdot \vec{E})\), which concerns electrical parameters, equals to zero. The initial director can be solved by means of the calculus of variations and finite difference method.

3.4. Initial Potential Calculation
The initial potential distribution can be calculated according to equation (2). It is critical for calculation to deal with boundary problems correctly, as are discussed below:

1) Liquid crystal / alignment layer interface: \(D_{n}^{LC} = D_{n}^{film}\). Upper alignment film / upper glass substrate interface: \(D_{n}^{film} = D_{n}^{glass}\). Where \(D_{n}^{LC}, D_{n}^{film}\) and \(D_{n}^{glass}\) are the normal component of electric displacement vector at interface in liquid crystal, alignment layer and upper glass substrate, respectively.

2) Top interface of glass substrate: \(E_{z} = -d\varphi / dz = 0 \) at \(z = 4d\), where \(d\) is the cell thickness.

3) Periodic boundary conditions: \(\frac{\partial A}{\partial X}\bigg|_{x=0} = \frac{\partial A}{\partial X}\bigg|_{x=N} \approx \frac{A(x = 1) - A(x = N - 1)}{2}\). Where \(N\) is the grid number of \(A\) divided in \(X\)-axis direction (\(A\) denotes director \(n_{i}\) or potential \(\varphi\)).

3.5. 2D Director Calculation and Results
Given the initial distribution of director and potential, 2D director can be solved according to equations (2), (3) and boundary conditions. For faster convergence and less error as possible, we employ finite difference method on non-uniform grids to calculate iteratively. The calculated potential and director distribution are illustrated in Figure 2 and Figure 3(a), respectively.

To decrease the influence of fringe field effect, we can increase the thickness of the upper alignment layer. The calculated director distribution is illustrated in Figure 3(b). It can be seen that non-uniform region 2 is smaller than region 1. In addition, decreasing the proportion of electrode gap to electrode width can also decrease the influence of fringe field effect.

4. Conclusion
A practical numerical model of LCOPA is set up based on its geometrical structure. 2D potential and director distribution in the cell are calculated by means of a finite difference method on non-uniform grids. Increasing the thickness of the upper alignment layer can decrease the influence of fringe field effect.
Figure 2. Calculated 2D potential distribution

(a) thickness of upper alignment layer is $0.1\mu m$

(b) thickness of upper alignment layer is $0.3\mu m$

Figure 3. Calculated 2D director distribution

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