Optik 126 (2015) 5269–5275

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.de/ijleo

Modeling of nematic liquid crystal cells subject to an externally applied field

M.A. Christou [a,*], A.C. Polycarpou [b], N.C. Papanicolaou [a]

[a] Department of Mathematics, University of Nicosia, 46 Makedonitissas Ave., 1700 Nicosia, Cyprus
[b] Department of Electrical and Computer Engineering, University of Nicosia, 46 Makedonitissas Ave., 1700 Nicosia, Cyprus

ARTICLE INFO

Article history:
Received 25 September 2014
Accepted 6 September 2015

Keywords:
Finite difference method
Nonlinear differential equations
Modal analysis
Mode-matching technique
Maxwell equations

ABSTRACT

A robust two-dimensional (2D) formulation for the electrical characterization of nematic liquid crystals (N-LCs) under low-frequency (LF) AC biasing conditions is proposed. The finite-difference (FD) method is first implemented to solve Poisson's equation in the domain of interest in order to obtain the governing LF electric field, which affects the local dielectric properties of the anisotropic material. Then, the nonlinear Euler–Lagrange partial differential equation (PDE), governing the orientation of the directors, is solved using one of three FD schemes with relaxation proposed in this paper. Once the N-LC layer is characterized, the average refractive index as a function of the *x*-coordinate is calculated assuming a normally incident monochromatic laser beam. The results are compared with published data in the literature obtained using a finite element method (FEM). Solution of the PDE governing the orientation of the directors in a non-uniform 2D electric field is obtained using either strong anchoring or soft anchoring. An investigation of the effects of boundary conditions on the average refractive index is presented.

1. Introduction

Liquid crystals are widely used in thin-film transistor (TFT) liquid crystal displays (LCDs) due to their attractive electro-optical properties [1]. As a result, TFT-LCD's completely replaced traditional cathode ray tubes (CRTs) in commercial applications. High-resolution displays though require pixels of small size, thus creating a strong fringing field near the edges of adjacent coplanar electrodes. This highly inhomogeneous low-frequency electric field with strong fringing effects near electrode edges creates disclination lines or defects which adversely affect the overall performance of the display. Specifically, the presence of disclination lines near electrode edges disturbs the electro-optical properties of the liquid crystal, thus reducing the contrast ratio and brightness of the display. The location of disclination lines is affected by the anisotropy of the crystal and the elastic constants [2]. Consequently, it is essential that accurate and computationally efficient numerical techniques are used for the characterization of LC's in the presence of a non-homogeneous low-frequency electric field.

Different numerical techniques have been proposed in recent years for modeling of LC's under a low-frequency bias electric field. The most common approach is to formulate an iterative process where the electric potential is solved for a given structure, and then, by using the obtained electric field distribution, one can solve for the directors' tilt angle in the domain of interest. A 2D hybrid finite element/finite difference numerical method based on a tensor formulation was used for the analysis of N-LC's cells in the presence of interdigital electrodes [3]. An improved steady-state analysis based on a finite-element formulation of the free-energy functional was implemented successfully for the analysis of 2D and 3D LC structures in the presence of a low-frequency field [4,5]. A similar finite-element approach was also implemented for the characterization of electromagnetic wave propagation in LC structures, at millimeter-wave frequencies, in the presence of a quasi-static electric field [6–8]. A Galerkin's FEM approach was also used to simplify the highly nonlinear governing equation in order to model the dynamic behavior of LC directors in complex structures [9]. A number of other numerical methods have been extensively used throughout the years for the analysis of LC's in the presence of an applied bias field.

Here, we propose an alternative numerical technique based on an iterative process where the electric potential and the director field are solved successively until convergence is reached. Solution of the directors' tilt angle in the domain of interest is obtained using one

* Corresponding author. Tel.: +357 22842515.
E-mail addresses: christou.ma@unic.ac.cy (M.A. Christou), polycarpou.a@unic.ac.cy (A.C. Polycarpou), papanicolaou.n@unic.ac.cy (N.C. Papanicolaou).

http://dx.doi.org/10.1016/j.ijleo.2015.09.016
0030-4026/

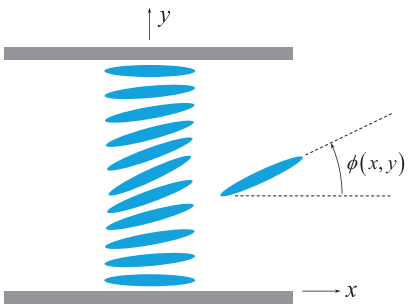

Fig. 1. Geometry of the a liquid-crystal cell showing the orientation of the directors with respect to the horizontal axis.

of three FD schemes with relaxation. The relevant FD schemes operate on the nonlinear PDE obtained using the Euler–Lagrange equation that minimizes the Oseen-Frank free energy functional [10]. The approach was implemented for a 2D problem, but can be extended to a generic three-dimensional (3D) structure.

2. Governing equations

The dielectric properties of the N-LC layer are directly related to the orientation of the directors inside the crystal. Under the assumption of z-invariance and in the absence of twist, the director orientation is defined by a unit vector in the xy-plane given by $\hat{n} = (\cos\phi, \sin\phi, 0)$, where the tilt angle ϕ is measured from the positive $x-$axis, as shown in Fig. 1. The response of the directors inside the crystal in the presence of a low-frequency electric field is governed by the Oseen-Frank free energy functional given by

$$\mathfrak{F} = \frac{1}{2}\int \left[k_{11}(\nabla\cdot\hat{n})^2 + k_{22}[\hat{n}\cdot(\nabla\times\hat{n})]^2 + k_{33}|\hat{n}\times(\nabla\times\hat{n})|^2 - \epsilon_0\left[\Delta\epsilon(\hat{n}\cdot\vec{E})^2 + \epsilon_\perp|\vec{E}|^2\right]\right]\mathrm{d}^3r, \tag{1}$$

where k_{11}, k_{22}, and k_{33} are the splay, twist and bend elastic constants of the crystal, and $\vec{E} = (E_x, E_y, E_z)$ is the electric field; $\Delta\epsilon = \epsilon_\parallel - \epsilon_\perp$, where $\epsilon_\parallel$ and $\epsilon_\perp$ are the relative permittivities of the crystal in the directions parallel and perpendicular to the director, respectively.

The functional $\mathfrak{F}$ in Eq. (1) can be minimized using the Euler–Lagrange equation

$$\frac{\partial f}{\partial\phi} - \frac{\partial}{\partial x}\frac{\partial f}{\partial\phi_x} - \frac{\partial}{\partial y}\frac{\partial f}{\partial\phi_y} = 0, \tag{2}$$

where

$$f = \frac{1}{2}\left[k_{11}(\cos\phi\phi_y - \sin\phi\phi_x)^2 + k_{33}(\cos\phi\phi_x + \sin\phi\phi_y)^2 - \epsilon_0[\Delta\epsilon(\cos\phi E_x + \sin\phi E_y)^2 + \epsilon_\perp(E_x^2 + E_y^2 + E_z^2)]\right], \tag{3}$$

and $\phi_x := \partial\phi/\partial x$ and $\phi_y := \partial\phi/\partial y$. Substituting (3) into (2), and manipulating the resulting terms yields

$$2(k_{11}\sin^2\phi + k_{33}\cos^2\phi)\frac{\partial^2\phi}{\partial x^2} + 2(k_{11}\cos^2\phi + k_{33}\sin^2\phi)\frac{\partial^2\phi}{\partial y^2} - (k_{11} - k_{33})\sin 2\phi\left[\left(\frac{\partial\phi}{\partial x}\right)^2 - \left(\frac{\partial\phi}{\partial y}\right)^2\right]$$

$$-2(k_{11} - k_{33})\left[\sin 2\phi\frac{\partial^2\phi}{\partial x\partial y} + \cos 2\phi\frac{\partial\phi}{\partial x}\frac{\partial\phi}{\partial y}\right] + \epsilon_0\Delta\epsilon[\sin 2\phi(E_y^2 - E_x^2) + 2\cos 2\phi E_x E_y] = 0. \tag{4}$$

The low-frequency (quasi-static) electric field in the structure is governed by Poisson's equation in a charge-free region:

$$\nabla\cdot(\hat{\epsilon}\nabla V) = 0, \tag{5}$$

where $\hat{\epsilon}$ is the relative permittivity tensor of the non-homogeneous crystal given by

$$\hat{\epsilon}(x,y) = \begin{bmatrix} \epsilon_{xx}(x,y) & \epsilon_{xy}(x,y) & 0 \\ \epsilon_{yx}(x,y) & \epsilon_{yy}(x,y) & 0 \\ 0 & 0 & \epsilon_{zz}(x,y) \end{bmatrix}, \tag{6a}$$

and

$$\epsilon_{xx} = \epsilon_\perp + \Delta\epsilon\cos^2\phi(x,y), \quad \epsilon_{xy} = \epsilon_{yx} = \Delta\epsilon\sin\phi(x,y)\cos\phi(x,y), \quad \epsilon_{yy} = \epsilon_\perp + \Delta\epsilon\sin^2\phi(x,y), \quad \epsilon_{zz} = \epsilon_\perp. \tag{6b}$$

Utilizing (5, 6) and assuming z-invariance, we obtain the equation governing the electric potential inside the LC:

$$\epsilon_{xx}\frac{\partial^2 V}{\partial x^2} + \epsilon_{yy}\frac{\partial^2 V}{\partial y^2} + 2\epsilon_{xy}\frac{\partial^2 V}{\partial x\partial y} + \left(\frac{\partial\epsilon_{xx}}{\partial x} + \frac{\partial\epsilon_{xy}}{\partial y}\right)\frac{\partial V}{\partial x} + \left(\frac{\partial\epsilon_{xy}}{\partial x} + \frac{\partial\epsilon_{yy}}{\partial y}\right)\frac{\partial V}{\partial y} = 0. \tag{7}$$

The electric field at a point in the crystal is computed by taking the gradient of the electric potential. The coupled system of equations (4, 7) will be solved iteratively until convergence is reached.