Analysis and model of the photorefractive-like effect in a non-conductive asymmetric liquid crystal hybrid cell

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Abstract—In this paper we describe a non-conductive liquid crystal hybrid cell with the photoconductive polymer (PP) layer. The orientation of the liquid crystal (LC) molecules in the described optical device is controlled by an external electric field and proper illumination. A method to calculate photoinduced refractive index distribution in the liquid crystal layer has been presented. We propose the model of a space charge formation in the photoconductive polymer layer in the presence of light. We assumed that the carriers generated by the light in the PP diffuse into an unlighted area and drift in an external field and local field of the generated charge. In determining the distribution of the space charge field, we take into account the field-induced charges on the borders of individual layers. After calculation of the final distribution of the space charge and proper field distribution, we determine the director field distribution and refractive index distribution in an LC layer.

The liquid crystal cell with a photoconductive polymer layer for controlling the liquid crystal layer is a structure that potentially allows laser beam steering and optical switching. In the cell, the light of small power can locally change the refractive index of the LC layer. This phenomenon is called a photorefractive-like effect and allows the formation of self-organizing LC fiber and its coupling [1, 2]. Photoconductive layer presence is crucial for light control. In literature, two influence mechanisms of a photoconductive polymer layer on a liquid crystal layer [3-7] are described. The first effect is the reduction of resistance of a PP layer and increase of the voltage drop across the LC layer. The second effect is the formation of a space charge due to localized illumination, which causes LC molecules movement.

In this paper, we present a three-step method to calculate refractive index distribution in a liquid crystal layer. In the first step the LC permittivity and field distribution inside the PP layer are calculated for a hybrid cell, which is only driven by external voltage (absence of a laser beam). In the second step, the space-charge distribution formed in a photoconductive polymer layer is calculated after the appearance of laser beam illumination. In this step, the transport and generation of carriers in the photoconductive polymer are described. In the third step, electric field distribution is determined with all previously determined components, and the refractive index distribution of the liquid crystal layer n_{eff} is calculated as well. This method takes into account the external driving voltage U, laser beam properties, LC and PP properties, and the configuration of a hybrid cell. All enumerated values have their own, particular impact on the final results.

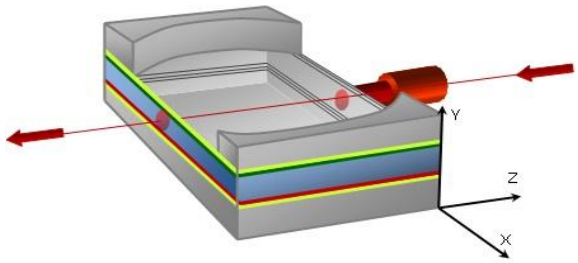

Fig.1. Propagation of a laser beam in an asymmetric hybrid liquid crystal cell consisting of glass (grey), ITO(yellow), photoconductive polymer (red), nematic liquid crystal (blue), ordering layer (green), ITO, glass.

Mathematical models and results were obtained for asymmetric hybrid cells in which the laser beam propagates along the liquid crystal layer. The analyzed cell is composed as in Fig. 1 and we assumed that the there was no carriers diffusion between individual layers. The current through the cell is zero. The LC molecules in an dark cell, and in the absence of external fields, have planar orientation. Furthermore, it is assumed that the hole's conduction strongly dominates in PP and that light intensity is distributed only in the direction perpendicular to the path of the laser beam (plane of incidence y–z).

The model used in the first step of the method describes a cell driven by an external field. It is based on equivalent circuit of liquid crystal cells, which assumes that the cell is a serial connection of capacitors representing different layers.

$$E_{EXT}^{LC} = U\frac{\varepsilon_{ol}\varepsilon_p}{\tilde{\varepsilon}_{LC}\varepsilon_p d_{ol}+\varepsilon_{ol}\varepsilon_p D+\varepsilon_{ol}\tilde{\varepsilon}_{LC}d}; \quad (1)$$

$$\frac{\varepsilon_0\Delta\varepsilon}{K}(E_{EXT}^{LC})^2 sin\theta cos\theta = \frac{\partial^2\theta}{\partial^2 y}$$
$$where:\ \theta(d) = \theta(d+D) = 0 \quad (2)$$

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$$\tilde{\varepsilon}_{LC} = \frac{D\varepsilon_{\parallel}\varepsilon_{\perp}}{\int_d^{d+D}\sqrt{\varepsilon_{\parallel}^2 sin^2\theta(y)+\varepsilon_{\perp}^2 cos^2\theta(y)}dy} \quad (3)$$

$$E_{EXT}^{p} = U\frac{\varepsilon_{ol}\tilde{\varepsilon}_{LC}}{\tilde{\varepsilon}_{LC}\varepsilon_p d_{ol}+\varepsilon_{ol}\varepsilon_p D+\varepsilon_{ol}\tilde{\varepsilon}_{LC}d} \quad (4)$$

$$U_s = U\left(1-\frac{\varepsilon_p\tilde{\varepsilon}_{LC}d_{ol}}{\tilde{\varepsilon}_{LC}\varepsilon_p d_{ol}+\varepsilon_{ol}\varepsilon_p D+\varepsilon_{ol}\tilde{\varepsilon}_{LC}d}\right) \quad (5)$$

In Eq. (1) the parameters ε_{ol}, ε_p mean the dielectric constant of material in the ordering layer (OL) and PP appropriately. While items d_{ol}, D, d represent the thickness of OL, LC and PP layers respectively. The equivalent circuit in place of the LC layer contains a variable capacitor because the permittivity $\tilde{\varepsilon}_{LC}$ depends on the electric field strength E_{EXT}^{LC}. The permittivity used to calculate the capacity of the capacitor is determined from the director field distribution θ in the LC layer. Equation (3) was derived assuming that the LC layer creates an infinite number of serial connections of capacitors with different permittivity. Director field distribution θ was obtained from the one-dimensional Euler-Lagrange equation for the liquid crystal [Eq. (2)].

Parameters $\varepsilon_{\parallel}$ and $\varepsilon_{\perp}$ are parallel and perpendicular dielectric permittivity of liquid crystal. Vacuum dielectric permittivity, dielectric anisotropy and Frank elastic constant for the liquid crystal are denoted by ε_0, $\Delta\varepsilon$ and $K=K_{11}=K_{22}=K_{33}$.

We assumed that the driving field influence and photoinduced charge field influence can be treated separately because of different response time for these two processes.

The formation of a photoinduced space charge was obtained by modifications to Schildkraut and Kukhtarev models that describe photorefractive materials [8-10]. The model includes the field of charges accumulated on the borders of PP/ITO and PP/LC formed under the influence of space charge in the PP and calculated by means of images method.

$$\frac{\partial p}{\partial t} = \frac{\partial N_A^-}{\partial t} - \frac{\partial T_H^+}{\partial t} + \frac{1}{e}div(\vec{j}) \quad (6)$$

$$\frac{\partial N_A^-}{\partial t} = \varphi I(x)(N_A - N_A^-) - \frac{\mu_p e}{\varepsilon_p\varepsilon_0}pN_A^- \quad (7)$$

$$\frac{\partial T_H^+}{\partial t} = r(T_H - T_H^+) - \gamma pT_H^+ \quad (8)$$

$$\vec{j} = e\left(\mu_p p\left(\vec{E}+\vec{E}_s\right) + \mu_p\frac{kT}{e}\nabla p\right) \quad (9)$$

$$\nabla\cdot\vec{E} = \frac{e}{\varepsilon_p\varepsilon_0}(p - N_A^- + T_H^+) \quad (10)$$

Transport, generation and recombination of carriers in the photoconductive material are described by the above system of equations. In accordance with the Langevin model we assumed that the speed of recombination is proportional to the concentration of holes p, ionized acceptors N_A^- and mobility of holes. Photogeneration efficiency ϕ is obtained from the Twarowski model [13]. It depends on the external field in the polymer layer E_{EXT}^{p}, and is anisotropic. Our model does not introduce the simplification of Schildkraut ($\phi\sim E^p$) [11,12], because the electric field used to drive LC cells is more than an order of magnitude lower than applied for charge driving in polymers used in the experiments by Schildkraut. In Eqs. (6)-(10) $I(x)$ is light intensity, r and γ denotes trapping and detrapping rates, μ_p denotes holes mobility, N_A and T_H are acceptors and traps concentrations, p, N_A^- and T_H^+ are the concentrations of holes, ionized acceptors and ionized traps, $\vec{j}$ means current density. Symbols k, e and T are the Boltzmann constant, electron charge and temperature respectively. Carriers mobility is selected from the model of Gill [14] and depends on the external field (E_{EXT}^{p}) and temperature. The charge density on the border PP/ITO $\sigma_{ITO\,/P}$ and PP/LC $\sigma_{P\,/LC}$ is calculated with the method of images for the charged wire (such a shape has the laser beam path inside the PP layer). This allows us to take into account the impact of charges along the beam path.

$$\sigma_{ITO\,/P}(x) = \int_{\alpha=-\infty}^{\infty}\int_{y=0}^{d}\frac{Q(x,y)}{2\pi\varepsilon_p((\alpha-x)^2+y^2)^{\frac{3}{2}}}dyd\alpha \\ \ldots + \int_{\alpha=-\infty}^{\infty} -\frac{\sigma_{P/LC}(\alpha)}{2\pi\varepsilon_p}\frac{y}{((\alpha-x)^2+y^2)^{\frac{3}{2}}}d\alpha \quad (11)$$

$$\sigma_{P\,/LC}(x) = \int_{\alpha=-\infty}^{\infty}\int_{y=0}^{d} -\frac{\tilde{\varepsilon}_{\mathrm{LC}}-\varepsilon_p}{(\tilde{\varepsilon}_{\mathrm{LC}}+\varepsilon_p)}\frac{Q(x,y)}{2\pi\varepsilon_p}\times \\ \times\frac{d-y}{((\alpha-x)^2+(d-y)^2)^{\frac{3}{2}}}dyd\alpha + \quad (12)$$

$$+\int_{\alpha=-\infty}^{\infty} -\frac{\tilde{\varepsilon}_{\mathrm{LC}}-\varepsilon_p}{(\tilde{\varepsilon}_{\mathrm{LC}}+\varepsilon_p)}\frac{\sigma_{ITO/P}(\alpha)}{2\pi\varepsilon_p}\frac{d}{((\alpha-x)^2+d^2)^{\frac{3}{2}}}d\alpha$$

$$Q(x,y) = e(p(x,y) - N_A^-(x,y) + T_H^+(x,y)) \quad (13)$$

After lighting the electric field in the cell is the sum of an external field and the field of space charge in the PP layer. For the constant value of an external field $\vec{E}_s$=(0, E_{EXT}^{p}), the system tends to a steady state in which all currents inside the PP layer are balanced.

$$\varepsilon_0 \nabla\varepsilon(y)\nabla V + \varepsilon_0\varepsilon(y)\nabla^2 V = -Q$$
$$\varepsilon(y) = \begin{cases} \varepsilon_p \text{ for } y \in (0,d) \\ \tilde{\varepsilon}_{LC} \text{ for } y \in \langle d, d+D) \end{cases} \quad (14)$$
$$Q = 0 \text{ for } y \in \langle d, d+D)$$
$$V(x,0) = V_1 \;\; V(x,d+D) = V_2$$

$$\vec{E} = -grad(V) = (E_x, E_y) \text{ for } y \in \langle d, d+D) \quad (15)$$

The field potential inside PP and LC is calculated from the Poisson equation [Eq. (14)]. The pre-calculated distribution of space charge in the PP layer has been exploited for this calculation. An additional voltage drop resulting from the appearance of space charge is applied to the LC layer. For the DC field, the distribution of space charge is constant and $|V_2 - V_1|$ is equal to the voltage drop across the LC layer and PP layer, presented as U_s.

The deformation of a liquid crystal layer is calculated in accordance with Eqs. (16). The resulting director field distribution allows for refraction index determination [15].

$$\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2} - 2cos2\theta\frac{\partial\theta}{\partial x}\frac{\partial\theta}{\partial y} =$$
$$\frac{\varepsilon_0\Delta\varepsilon}{K}\left((E_y^{LC})^2 - (E_x^{LC})^2\right)sin2\theta - \frac{\varepsilon_0\Delta\varepsilon}{K}E_x^{LC}E_y^{LC}cos2\theta \quad (16)$$
$$\text{where } \theta(x,d) = \theta(x,d+D) = 0$$

$$n_{eff}(x,y) = \frac{n_\parallel n_\perp}{\sqrt{n_\parallel^2 sin^2\theta(x,y) + n_\perp^2 cos^2\theta(x,y)}} \quad (17)$$

Equations (16) have been received for the LC where $K=K_{11}=K_{22}=K_{33}$. When the elastic constants are not equal, equation (16) will be more complicated. Strong anchoring has been assumed in boundary conditions for director field calculation.

Figure 2 illustrates the results obtained with the method described in the article. The space charge is formed by diffusion into the dark area and screening of an external field in the PP layer. Homeotropic orientation was achieved by applying an external voltage. In the illuminated area, homeotropic orientation is stronger, due to the additional field of a photoinduced space charge. Particular director's field distribution is obtained inside the illuminated area along the light beam path. During the calculations we have used a finite difference method. The thickness of the photoconductive layer and the polyimide polymer is 100nm, and the thickness of the liquid crystal layer is 5μm. The photoconductive polymer used in the calculation corresponds to a mixture of PVK: TNF in a molar ratio of 1: 0.2. The parameters of the liquid crystal mixture are: n_e=1.9, n_o=1.55, $\Delta\varepsilon$=5, K=6·10^{-12}N, U=6.4V. The power of the laser beam is 0.5mW and Gaussian beam distribution has been assumed for calculations.

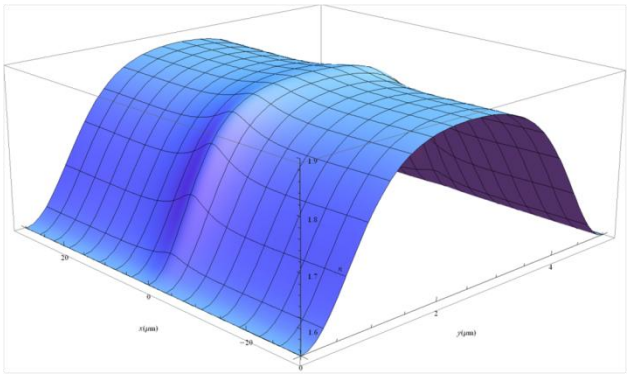

Fig. 2. Refractive index distribution in a liquid crystal layer for AC driving voltage.

The presented paper explains the way to calculate numerically the phenomena inside an LC hybrid cell with photoinduced conductivity in one aligning layer. Mathematical models of phenomena occurring in the liquid crystal cell hybrid constructed for proper numerical calculation are shortly described. Details for space charge calculations are to some extent new and allow for potential $V(x,y)$ distribution inside the LC layer. Finally, one obtains an opportunity to analyze how the parameter of layers influences the behavior of a complex optoelectronic device.

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