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Semiconductor–LC Layer Boundary and Photonic Structures

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Theoretical discussion and numerical results for experimentally obtained new kind of the optical waveguide has been presented. Discussed waveguide is optically self-induced during light beam propagation along boundary between liquid crystal and semiconducting polymer. Light is propagated in electrically driven liquid crystal (LC) cell. Experimental results obtained earlier are reported in here shortly, and theoretical model of the observed phenomena is discussed as well as numerical outcome. Exploited nematic liquid crystal was of high birefringence near to 0.35. Experimental data have been obtained in the case of poly (N-vinyl) carbazole as photorefractive polymer doped with 2, 4, 7-trinitro-fluorenone, and numerical simulation has been done for this case.

Keywords Liquid crystal; organic semiconductor; self-guidance; waveguide

1. Observed Phenomena and Research Motivation

Optical waveguide structures obtained by means of optical induction in a thin LC film driven between two photo-chromic commands surfaces have been reported earlier by other authors [1]. This solution applies Langmuir-Blodgett-Kuhn monomolecular layers of a polymer with azobenzene side chains deposited on a glass sheet. When exposed to light of appropriate wavelength, the command surfaces undergo the trans-cis photo-isomerization process that induces a reversible change of orientation in the lc layer situated next to the command surface. Such change of the LC layer orientation can create an optical waveguide along way of an external beam illuminated monomolecular layer. The transition induced in LC layer is shown to be continuous, depending on the ratio of the cis-trans chromophore concentration in the command surface. Some kind of disadvantage is there because of the waveguide, and light beam, which induces wave-guiding path, are not co-planar and cannot be arranged in an integrated device. More innovative way seems to be nonlinear waveguides array first introduced by Christodoulides et al. [2]. This concept has been widely developed by Assanto, and also by Assanto and Karpierz et al. [3], and also in other work of Assanto and co-workers. Authors used an interaction of a laser beam with the LC layer driven by patterned electrodes forming light guiding channels. Unfortunately it yet seems be quite

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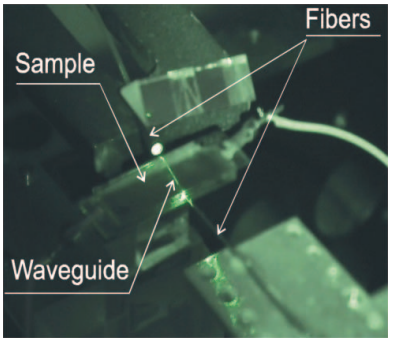

Figure 1. Experimental observation of the self-induced waveguide [8].

away from present fiber net technology. We are looking for possibility to design such solution, which could be applied in present fiber net technology.

In reference to mentioned results we observed the waveguide creation in the case when electrically driven LC layer aligned on photoconductive polymer (see Fig. 1) and common polyimide on the opposite side of the LC cell interacts with light beam propagated along boundary between aligning layers and LC. Observed light beam is guiding at very long distance (∼15mm) across LC cell with no observed and possible to measure beam widening due to refraction (see Fig. 1). It indicates that light creates the waveguide for itself, and no self focusing of light is observed as is reported in previously cited literature [3]. Because of good transparency of liquid crystal in all visible range up to near infrared spectrum the dominant losses during propagation are scattering losses. Good aligning of the LC in the strong electric field (range of 10^6 V/m) causes that we can assume scattering on number of optical heterogeneities of the LC layer as relatively small. Experimental results have been presented and discussed earlier [4].

Fibers ended with focusers (indexed 1 in the Fig. 2 and visible in Fig. 1) are placed on a stage controlled by piezo-actuators with submicron accuracy of step, and have been explored as tools for light beam insertion and dropping into and from LC layer. Upper side of the sample was transparent and light beam path was registered by means of zoomed CCD camera. Observations have been done in crossed polarizers. One polarizer is placed under LC cell while the second polarizer has been placed on the camera. The laser beam path in the sample has been shown schematically in the Fig. 2, and its experimental observation in Fig. 1. The cells before measurement were kept in the dark while short series of DC pulses of amplitude 5 volts has been applied to remove charged impurities from the bulk of LC layer. All measurement has been done in carefully controlled temperature near to 22°C. We observed, that there exist most preferred guided light polarization and it is perpendicular to the plane of the LC layer it means propagated light beam is p-polarized. With assumed coordinates we can call it p-polarized while zy-plane is the plane of beam incidence (Fig. 2). There is no beam widening due to refraction inside LC layer. Such beam refraction could be expected because of uniformity of the nematic layer driven by an external voltage. Explanation is that this LC layer uniformity has to be disturbed locally along beam path and properly polarized light is guiding along the disturbance. After light and external voltage have been turned off one can observe the path shadow, which remains steady. Registered deformation is an evidence of the localized electrostatic interactions between photoconductive polymer and liquid crystal in the previously illuminated area. The experiments have been performed for laser wavelengths equal to 532 nm and 638,

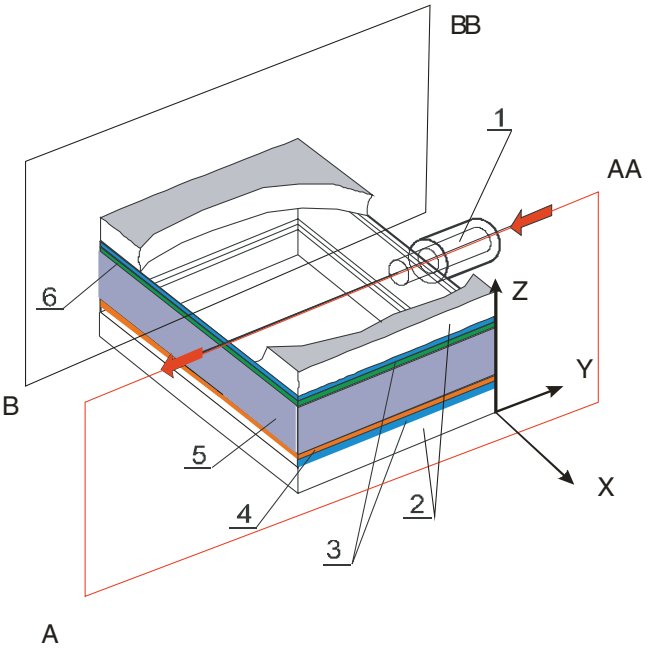

Figure 2. Liquid crystal cell arrangement in the experiment with asymmetric aligning layers. 1-fiber with focuser, 2-glass plates, 3-ITO electrodes, 4,6-aligning layers of polyimide (6) and PVC (4), 5-LC layer. Coordinates x,y,z as well as cross-sections A-AA, and B-BB added for results and discussion clarity [4]. Light propagates in A-AA cell cross-section.

2 nm. In both cases we get the waveguide and waveguides coupler [4]. The presence of the driving voltage is necessary to get a waveguide creation. The DC voltage polarized with +(ITO/PVC/LC/PI/ITO)- is most effective in the waveguide formation. For opposite DC voltage polarization the waveguide has not been observed. This asymmetric behavior probably indicates the presence of the junction between semi-conducting PVC and isolating LC. It suggests also mono-carriers conductivity in doped polymer.

The scheme of the LC cell shown in Fig. 1 as the sample has been placed in Fig. 2.

Aligning of liquid crystal with photopolymer has been reported in literature [5–7]. To mention a few. Nevertheless our experimental results are theoretically analyzed and model has been built proper for further simulations. It seems lack of such analysis yet in literature especially for the case of light interaction with hybrid devices contained semiconductor-LC layer.

2. Theoretical Background

2.1. Discussion of Space Charge Field Excited in Illuminated Organic Semiconductor

It is not clear yet if long standing discussion whether the primary photo excitations in conjugated polymers should be described in terms of a semiconductor band-structure or as molecular excitons points out which way is more effective [8,9,10, and 15]. Though some conjugated polymers behave as well-ordered bulk semiconductors, many of them are usually more disordered materials [11,17,12,13].

We want to propose more phenomenological model to exploit well defined and possible to measure characteristics of photosensitized polymer such as charge mobilities, dopant density, and so on. Let us assume most obvious phenomenological model well known from semiconductor theory:

$$\begin{aligned}
\frac{\partial \mathrm{n}}{\partial \mathrm{t}} &= (g_{n0} + \mathrm{g_n I(x)})(\mathrm{N_D} - \mathrm{N_D^+}) - \gamma_\mathrm{n} \mathrm{n N_D^+} - \mu_\mathrm{n} \mathrm{n} \frac{\partial \mathrm{E}}{\partial \mathrm{x}} - \mu_\mathrm{n} \mathrm{E} \frac{\partial \mathrm{n}}{\partial \mathrm{x}} + \mu_\mathrm{n} \mathrm{k_B T} \frac{\partial^2 \mathrm{n}}{\partial \mathrm{x}^2} \\
\frac{\partial \mathrm{N^+}}{\partial \mathrm{t}} &= (g_{n0} + \mathrm{g_n I(x)})(\mathrm{N_D} - \mathrm{N_D^+}) - \gamma_\mathrm{n} \mathrm{n N_D^+} \\
\frac{\partial \mathrm{p}}{\partial \mathrm{t}} &= (g_{p0} + \mathrm{g_p I(x)})(\mathrm{N_A} - \mathrm{N_A^-}) - \gamma_\mathrm{p} \mathrm{p N_A^-} + \mu_\mathrm{p} \mathrm{p} \frac{\partial \mathrm{E}}{\partial \mathrm{x}} + \mu_\mathrm{p} \mathrm{E} \frac{\partial \mathrm{p}}{\partial \mathrm{x}} - \mu_\mathrm{p} \mathrm{k_B T} \frac{\partial^2 \mathrm{p}}{\partial \mathrm{x}^2} \\
\frac{\partial \mathrm{N^-}}{\partial \mathrm{t}} &= (g_{p0} + \mathrm{g_p I(x)})(\mathrm{N_A} - \mathrm{N_A^-}) - \gamma_\mathrm{p} \mathrm{p N_A^-} \\
\frac{\partial \mathrm{E}}{\partial \mathrm{x}} &= \frac{\mathrm{q}}{\varepsilon}(\mathrm{N_D^+} - \mathrm{N_A^-} + \mathrm{p} - \mathrm{n})
\end{aligned} \tag{1}$$

Where: I(x) is light intensity, g denotes generation coefficient for appropriate carriers, γ denotes recombination coefficients for appropriate carriers, μ denotes appropriate carriers mobility, $\mathrm{N_A}$ and $\mathrm{N_D}$ are donors and acceptors concentrations, E means electric field of carriers which finally creates space charge field, p and n are number of excited carriers.

Because of very thin photoconductive polymer layer one can assume one dimensional equation for charge behavior inside this layer. Simple immediate analysis of that provide well known Kukhtarev model [14] for space charge field when we assume that all charge excitation and recombination are just near thermodynamic balance condition. Than:

$$E^{sc} = \frac{k_B T}{e} \frac{1}{I(x)} \frac{dI(x)}{dx} \tag{2}$$

Unfortunately such model does not allow designing effective model of photopolymer during further calculations because neglecting of carriers transport around illuminated area. Therefore numerical calculation just from equations of full phenomenological model (1) seems to be the best way to obtain space charge field then Kukhtarev model. Result dependent on charge mobilities, dopant molar ratio, generation and recombination coefficients are illustrated in figures below. From well known work of Gill [15] we know, that molar ratio of dopant determines mobilities of carriers up to change of conductivity of carriers from holes to electrons. So one can expect, that space charge field provided from (2) should be dependent on concentration of dopant N+ and N−. Also g versus γ ratio will influence this field. Only when dopant causing charge transfer in polymer behaves like pure acceptor or pure donor one can expect that space charge field will arise. It is to some extent sophisticated because of charge transfer mechanisms that causes conductivity of photo-sensitized polymer. Model shown in (1) is not direct charge transfer model. Yet it allows analysis of carrier movement and space charge field estimation also when proper dopant causes carrier movement possible by means of charge transfer. Dopant concentration is then obtained from molar ratio of photo sensitizer [15]. Results for space charge field have been shown in the Fig. 3. Shape of the field has been calculated for molar ratio of dopant which ensures hole like conductivity in doped polymer. Distances in Fig. 3 are shown around the centre of the light beam.

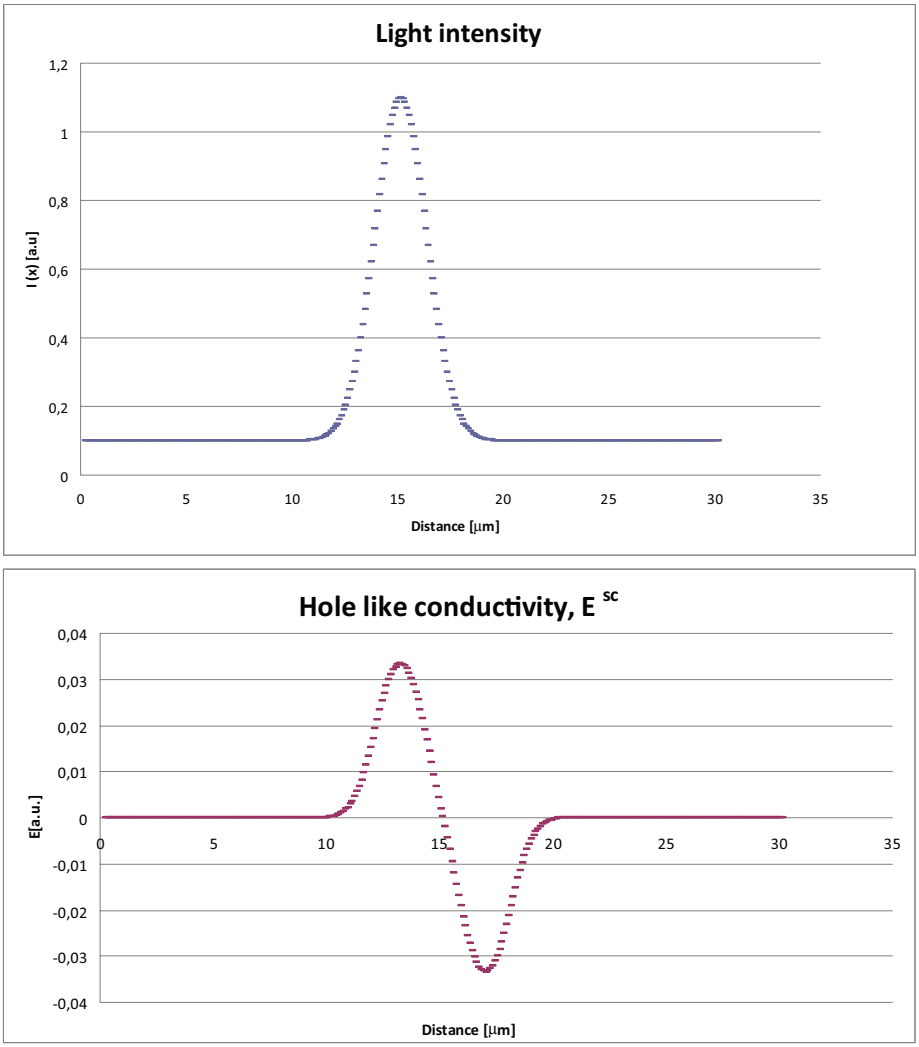

Figure 3. Shape o the space charge field inside photosensitized polymer layer caused by a light beam above (Gaussian like beam, dopant molar ratio: 20:02).

2.2. Oseen-Frank Equations and Model for LC Layer Deformation

Deformation of director field in examined liquid crystal layer undergoes Oseen-Frank equation in the form:

$$\frac{\partial^2\Theta}{\partial x^2}+\frac{\partial^2\Theta}{\partial z^2}-2\cos 2\Theta\,(x,z)\,\frac{\partial\Theta}{\partial x}\frac{\partial\Theta}{\partial z}=\frac{\varepsilon_0\Delta\varepsilon}{K}\left(E_z^2-E_x^2\right)\sin 2\Theta\,(x,z)$$
$$-\frac{\varepsilon_0\Delta\varepsilon}{K}E_xE_z\cos 2\Theta\,(x,z) \tag{3}$$

So called one Frank constant approximation has been applied in the equation. Sample geometry used during experiment allow us to say, that in the first approximation one can

assume an external AC driving field as E = (0,0,E_z) while electrostatic, photo-induced space charge field inside photopolymer layer is composed as E = (E_x,0,0). For simplicity we neglect screening of this field by carriers inside LC layer during space charge excitation. Screening charge can be described in terms of mirror charge condition:

$$\sigma_{pol} = -\frac{q^{sc}}{2\pi}\frac{\varepsilon_{AL} - \varepsilon_{eff}}{\varepsilon_{eff}\left(\varepsilon_{AL} + \varepsilon_{eff}\right)}\frac{d_g}{\left(\rho^2 + d_g^2\right)^{3/2}} \tag{4}$$

Proper effective permittivity is described as:

$$\varepsilon_{eff} = \sqrt{\frac{\varepsilon_{//}\varepsilon_{\perp}}{\varepsilon_{//}\sin^2\Theta(x,z) + \varepsilon_{\perp}\cos^2\Theta(x,z)}} \tag{5}$$

The ε_{AL} is dielectric permittivity of the aligning layer of photosensitized polymer, ε_{eff} is the effective dielectric permittivity of the nematic LC calculated here with the use of angle Θ(x, z) which should be obtained from (3) unfortunately. Item d_g is the induced charge layer thickness which can be assumed as photopolymer layer thickness as well, and q is the value of the photo-induced charge. The distance ρ is measured in plane of the photosensitized polymer layer. So field of this charge causes screening of space charge field inside LC layer. One can see that phenomenological model of all LC cell behavior during light propagation seems to be quite complicated and our calculations should be self-consistent.

After some algebra and numerical self-consistent calculation one can predict the LC layer deformation in examined electric fields as in the Fig. 4. Initial nematic LC layer alignment was planar. It means that localized space charge causes additional and localized deformation of the LC layer just along CW (Continuous Wave) laser beam propagation. Because of refractive index in this deformation area is generally higher than in its vicinity so light excites guided modes in this area. It is higher for p-polarized light beam propagating in

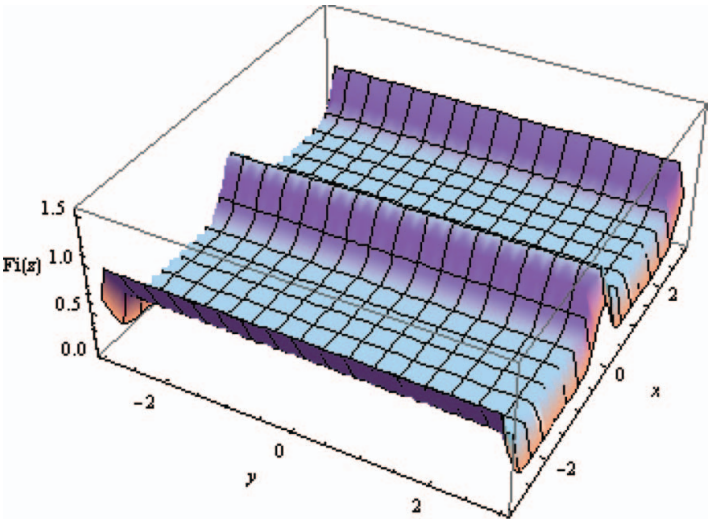

Figure 4. Numerical result for LC layer localized deformation along CW light beam path. Exposed distances value is measured in micrometers. (x, y, z axes the same as in Fig. 2: Fi (z)–director field rotation angle across the LC layer obtained from formula (3), y–along light beam propagation, x–along entrance edge of LC cell).

uniaxial LC layer. So conditions for self-guidance of light have been fulfilled. For LC data $n_e = 1.9$, $n_o = 1.55$, $\Delta\varepsilon = 5$, K = $6^{*}10^{-12}$ N, driving voltage $U_{rms} = 6.4$V, and light power $P = 0.1$mW obtained shape of refractive index in LC layer along light path has been shown in the Fig. 4. Width of the photo induced channel depends on permittivity of LC, permittivity of photosensitized polymer, molar ratio of dopant in PVK, driving voltage range.

3. Summary

Mechanisms of the light self-guidance in liquid crystal cell aligned with common polyimide aligning layer on the one side of the cell and photosensitized polymer on the second side has been explained. Described phenomena are different from known soliton like self-focusing of the light during propagation along in LC cell. Obtained results has been observed experimentally earlier and published in 2008 [4]. Here theoretical models as well as some numerical results have been presented after research of different LC cell and photorefractive aligning layers. We tried to build obvious phenomenological model to explain quite complicated problem.

Proposed models include photosensitized material data and allow one prepare simulation which describe behavior of the photo-induced waveguide in dependency on such material data as well as LC layer data. Simultaneous simulation of whole hybrid cell contained LC layer and photosensitized polymer as aligning layer seems to be reported for the first time. Rather speculative character of analysis presented in literature up to now does not provide full device simulation. Presented results can be assumed as integrated simulation way for hybrid, semiconductor-LC layer cell behavior during external field driving, and light beam interaction in LC cell.

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