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COMPUTER SIMULATION OF THE PULSE-PERIODIC ELECTRIC FIELD EFFECT ON THE 2D DIRECTOR ORIENTATION OF NEMATIC LIQUID CRYSTAL. EXPERIMENTAL RESEARCH OF MULTIMODE NEMATIC LIQUID CRYSTAL WAVEGUIDES

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Abstract. In this paper, we numerically investigate a two-dimensional differential equation describing the motion of a director of a nematic liquid crystal for the case of an alternating external electric field. The presence of the previously discovered accumulation effect has been confirmed by numerical modeling. A comparison is made with the case of a constant electric field, and also a qualitative comparison with an experiment is given. Incomplete agreement with experimental data indicates the need for further research. However, it should be noted that the constructed mathematical model of the phenomenon allows at this stage to obtain estimates that are sufficiently acceptable for experiment and correctly predict the dynamics of processes in liquid crystals. An analysis of the features of the propagation of quasi-waveguide modes in a liquid crystal waveguide showed that, in the case of dynamic processes, such effects as power exchange between coupled modes, leakage of modes, re-emission of modes into modes of a different order, etc., can be observed. The programs for numerical solution and computer modeling of two-dimensional parabolic partial differential equation were developed both in FORTRAN and C/C++.

The results obtained are important for further investigation of dynamic processes inside non-stationary liquid crystal layers, both from a theoretical point of view for understanding kinetic processes in liquid crystals and from a practical point of view when organizing and conducting different experimental research.

Keywords: liquid crystal, director, 2D fluctuations, irregularities, boundary-value problem, optofluidics, waveguide, laser radiation, numerical simulation.

1. Introduction

The establishment of the basic relationship between the properties of *liquid crystals* (LCs) and their structure [1-17] is important for various applications. The research in this field includes the development of a theoretical model for the object under study, considering its response to external actions (electric or magnetic fields, light, etc.), and correct interpretation of experimental data (in particular, using mathematical modeling and computer simulation).

The importance of these studies is determined by the practical application and prospects of these materials in high-speed low-energy LC data imaging devices; low-cost organic light-emitting displays and solar cells; and integrated optical devices, for example, coupling elements, modulators, distributed Bragg reflectors, sensors, processors; and is also perspective for optofluidics applications (see e.g. [17-21]). Additionally, some of the results of these studies may be useful when researching, for example, such an effect as the second harmonic generation (SHG) [12].

Although the fact that the phenomenon of the change in the director orientation of an LC in electric and/or magnetic fields has been studied in detail for static and slowly varying fields [1-5], the research of this phenomenon in a pulsed-periodic electric field is of practical interest [11-13]. We should note that in the paper [11] the time dynamics of the director of the *nematic liquid crystal* (NLC) in the field of a sequence of rectangular pulses was studied but for another cell configuration and lower electrode voltage.

In the paper [16] some results of the simulation of the static electric field effect on the director orientation of nematic liquid crystal were presented. We should note that in this study, the effect of introducing time dependence into the two-dimensional differential equation describing the NLC director motion in a dc electric field was analyzed [16]. At the same time, there is a practical need to study various behaviors when there is a real dependence of the director orientation of an LC on the time, for example when the high pulse-periodic electric field is applied in the experiments.

2. LC cell structures

Let us consider the 2D LC cell shown in fig. 1 (side (*a*) and end (*b*) views). To be specific we consider the cell with side electrodes [12, 13]. The cell's walls are glass plates. NLC had a homogeneous planar orientation with an optical axis along the direction of the director (coincides e.g. with the axis z). In another case, the internal surfaces are covered with surfactant which creates a homeotropic (θ = 90°, fig. 1(*b*)) orientation of an LC. The director orientation $\mathbf{n}$ was determined by the angle $\theta(x, y; t)$ between the vector $\mathbf{n}$ and y axis (see fig. 1(*b*)).

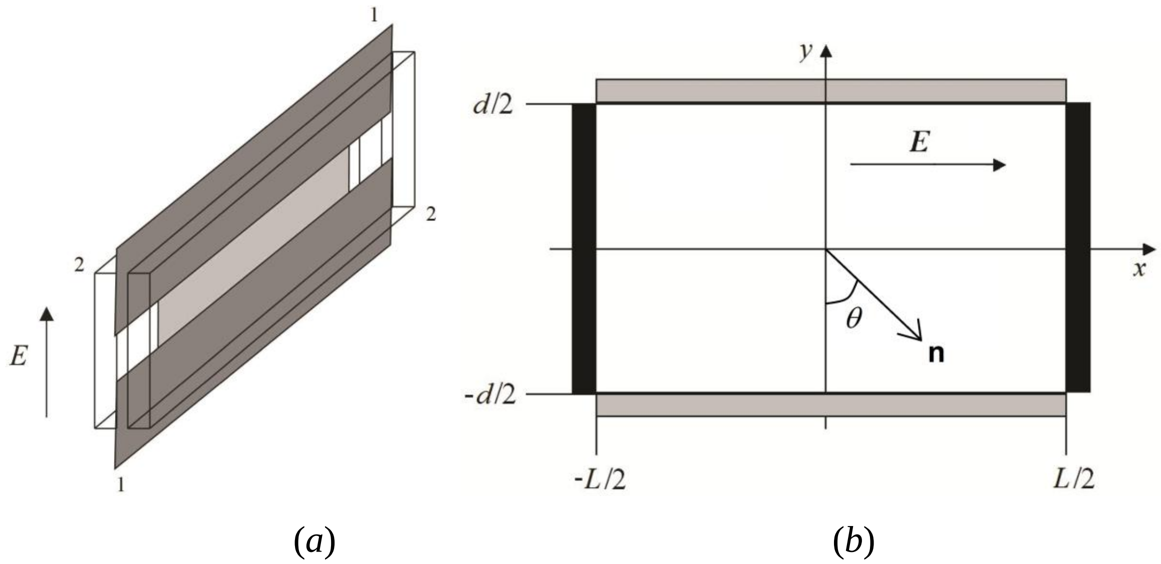


Fig. 1. Schematic representation of the LC cell: (*a*) – side view; (*b*) – end view.

The objects of the study are the NLC cell (fig. 1) formed from NLC 4-Cyano-4'-pentylbiphenyl (4-Cyano-4'-pentylbiphenyl or 5CB), well known from publications in the scientific and scientific literature (see e.g. [1-18]). In this geometry, the equation of director motion, which expresses the balance between the elastic and viscous torque and the external field torque, has close-to-zero initial and boundary conditions.

Schematic of the LC cell (see fig. 1): 1 – metal (copper foil) electrodes; 2 – glass plates (LC layer is inserted between glass plates); E indicates the direction of external pulsed-periodic electric field; d is LC layer thickness; L is distance between copper electrodes, L was about $2{\cdot}10^{-3}$ m.

The LC cell with different thicknesses (25, 75, and 125 μm) were studied in experiments, but the main part of the results was given only for the LC cell with $h \approx$ 125 μm. A high-voltage pulse (repetition frequency of about 10 Hz) was applied to them.

3. Theory and experiment. Results of computer modeling

The external electric field E is directed along the y axis. Let us assume that only the longitudinal and lateral bendings of the LC director arise due to the electric field action, while the change in the director's orientation (the LC's deformation) is determined only by the balance between the moments of the electric field and elastic forces. In our case, the LC director orientation is determined by the angle θ between the vector $\mathbf{n}$ and y axis.

Due to the anisotropy of the diamagnetic and dielectric susceptibilities, the free energy of the ensemble of NLC molecules in the external electric (or magnetic) field has a minimum at a well-determined (preferred) orientation of the molecular axes (the director) relative to the field (see e.g. [1, 2]). If the directions of the field and director in the initial state do not satisfy the condition of the minimum of the free energy at quite a high field which is capable of overcoming the NLC's elastic forces, the director will be reoriented and its new stationary distribution will be established. This effect was discovered and investigated in detail by Frederiks with his colleagues in the 1930s [1-6]. The electro- and magneto-optical effects specific of liquid crystals are caused by reorientation of the LC director (which determines the direction of preferred orientation of molecules in a macroscopic volume of material) under action of field or liquid flow.

In our previous paper when carrying out the standard minimization procedure for the free energy of the ensemble of NLC molecules [15] in the external electric field E and not going beyond the qualitative estimation of the final results to simplify the problem's solution, we obtained the second-order partial differential equation [12, 15, 16, 18, 21]. Then the numerical solutions of this equation with known boundary conditions were obtained and studied. The boundary-value problem and obtained second-order partial differential equation were approximated by well-known finite-difference schemes [22]. To accelerate the iterative processes, control of the accuracy of the obtained solutions and precision of the results, the calculations were carried out on a sequence of grids. The programs for solving the boundary-value problem were realized in FORTRAN and C/C++ [12, 15, 16, 18, 21, 22].

The results of the numerical modeling showed that the considered two-dimensional model with a constant electric field varying within wide limits did not allow us to give a complete explanation of the effect observed in the experiment with 2D LC cell [12, 13, 15, 16], which apparently is conditioned by the pulse-periodic character of the applied electric field [15] and 2D character of the Frederiks's effect [16-18, 21]. Note that we didn't take into account other possible effects, e.g. hydrodynamic processes or some possible inhomogeneity of the initial distribution of LC molecules over the cell volume especially in the irregular border areas [1, 2, 4, 8, 9]. The combination of these effects can lead to deviations from the results obtained by numerical modeling, some of which are presented below. At the same time, the results obtained reflect the main features of the studied phenomenon.

1D and 2D models of Frederiks effect were used for the analysis of the electric field effect on LC director orientation in the cell with the homeotropic orientation that helped us to understand the behavior of the nematic liquid crystal under study. Corresponding partial differential equation of the second order can be written in the next form [12, 15, 16, 18, 21]:

$$4\mathrm{K}\left(\theta_{xx}+\theta_{yy}\right)+\frac{1}{2}\varepsilon_0 \Delta\varepsilon E^2 \sin 2\theta = 0, \quad (1)$$

where the constant $K=\left(K_{11}+K_{33}\right)/2$, and appropriate elastic modules are equal, respectively: K_{11} = 7·10^-12^ N, K_{33} = 10·10^-12^ N; ε_0 = 8,854·10^-12^ F/m is vacuum electric constant; $\Delta\varepsilon$ = 14 is dielectric constant anisotropy; $\theta_{\alpha\alpha}=\partial^2\theta/\partial\alpha^2$, $\alpha = x, y$. In Eq. (1) $E=E(t)$ is the external pulse-periodic electric field that had a period T_0 =

0.1 s; in the beginning of each period (during the time interval ≈ 10^{-5} s), $E(t) \approx 10^6$ V/m, whereas during the rest of the period the field was zero.

The boundary conditions were specified as:

$$\left.\begin{cases} \theta(x, \pm d/2) = 0 \\ \theta(\pm L/2, y) = \pi/2 \end{cases}\right\}, \tag{2}$$

where d is LC layer thickness, $d = 10^{-4}$ m; L is distance between electrodes, $L = 2 \cdot 10^{-3}$ m.

The solutions to Eq. (1) with boundary conditions (2) are sought within the cell specified region: $-L/2 \le x \le L/2$ and $-d/2 \le y \le d/2$, at $L = 2 \cdot 10^{-3}$ m and $d = 10^{-4}$ m. Conditions (2) are determined by the value of the energy of the cohesion of molecules with the cell surface.

Frederiks transition threshold for the central part of the cell, as well as dependencies of the distribution of the director orientation on the high electric field, have been obtained. The results of the numeric calculations for different cases have been compared to the experiments (see e.g. [12, 13, 15, 16-18, 20, 21]).

As one example in fig. 2 depicted 2D director dynamics in the investigated 5CB NLC cell for the case described by the equation (5), where pulse-periodic electric field had the form $E(t) \approx 10^6 e^{-at} \sin(\pi t / b)$ ($E \approx 10^4$ V/m is considered as the Fredrik's effect threshold for the deformation of a two-dimensional LC director by a constant electric field [15]), and parameters $a = 2 \cdot 10^5$, $b = 10^{-5}$, for three periods of the field $E(t)$ since time 0 s, i.e. one can observe accumulation effect during 0.3 s in total (for more information about experimental conditions see e.g. [12, 13, 20]). In the beginning, one can see the initial $\theta(x, y; t)$ distribution.

Fig. 3 shows the difference of $\theta(x, y; t)$ distributions for the periods with $t = 0.3$ and 0.1 *s*, which confirms the accumulation effect [12, 13, 15, 16, 20, 21]. A more detailed analysis of the obtained results is beyond the scope of this work since the main goal was to demonstrate the efficiency of the developed algorithms and programs for the numeric analysis of the phenomenon under study.

Comparison of the figures given in the present paper with figures from works [12, 13, 20, 21] showed that the two-dimensional model quite accurately reflects the previously discovered accumulation effect, both within each period T_0 and within several periods T_0 [11, 12]. Moreover, the saturation angle $\theta_{max} \to 80^\circ$ and is reached in about several minutes what was established earlier in 1D models [12, 13, 20, 21].

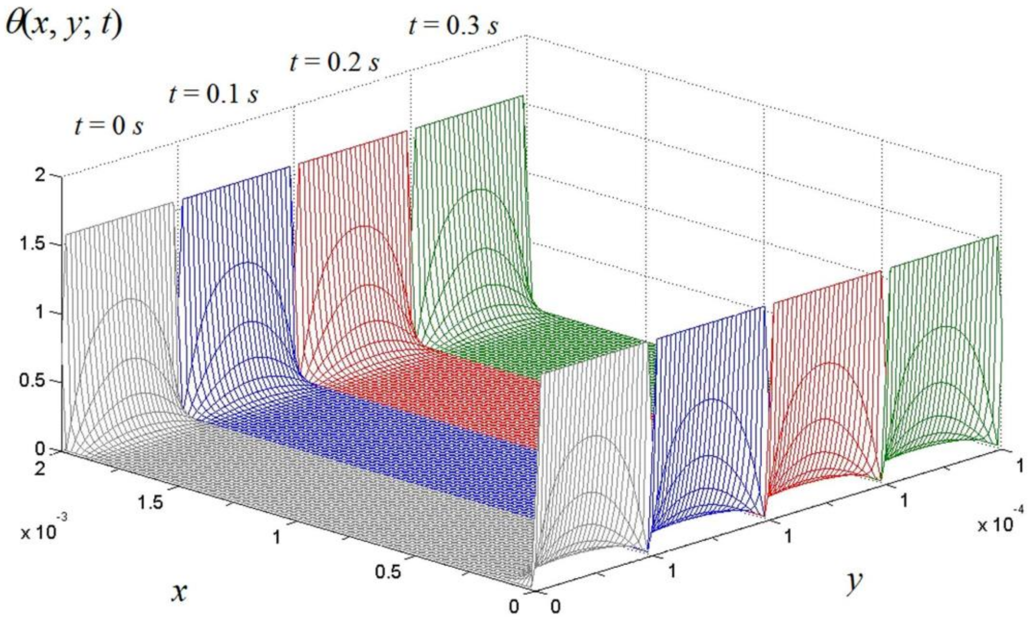
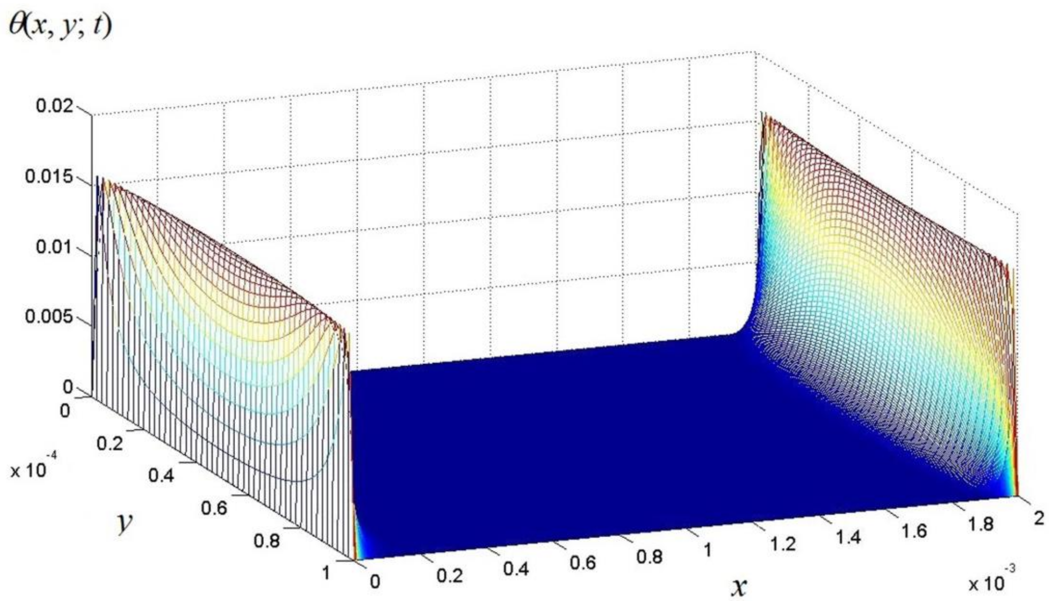
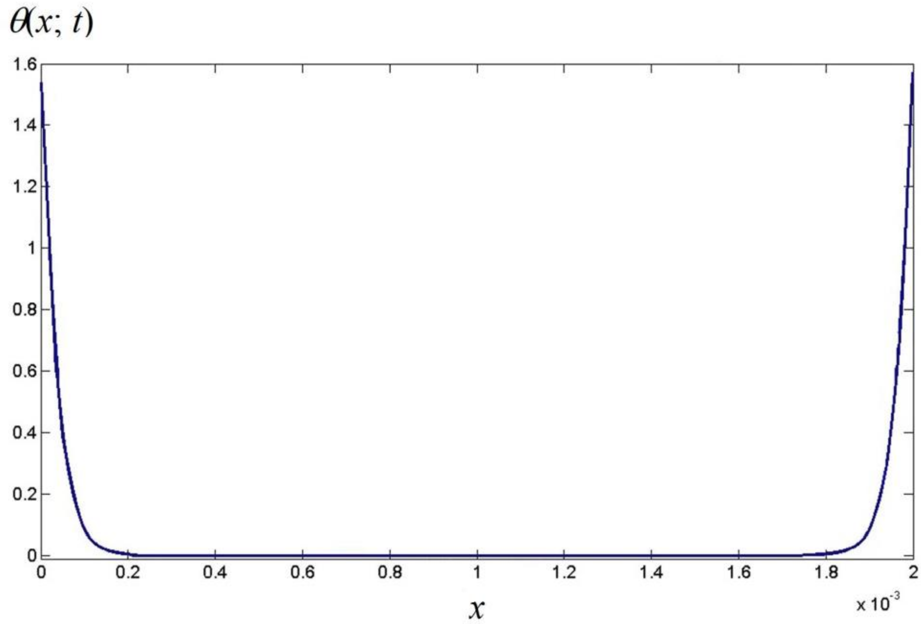


Fig. 2. 2D director dynamics in 5CB NLC cell for three periods, when external pulse-periodic electric field $E >> 0$. $L = 2 \cdot 10^{-3}$ m.



(a)



(*b*)

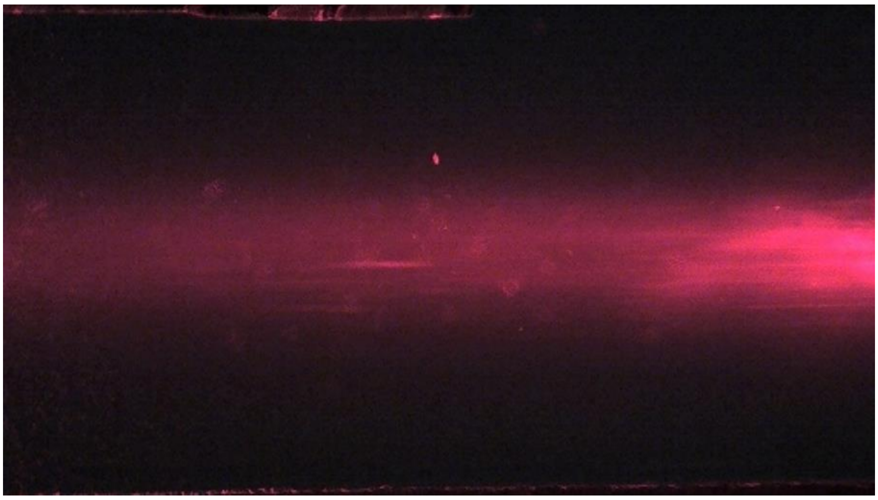
Fig. 3. Director dynamics in 5CB NLC cell when external pulse-periodic electric field $E >> 0$; the same as on fig. 3(*a*) but only for x coordinate when $y = 0.5 \cdot 10^{-4}$ cm; t = 0.1, 0.2, 0.3 s.

The main conclusions are as follows. The maximum deflection of the angle θ is achieved at the center of the cell, i.e. $\theta(d/2, L/2) \to \theta_{\max}$, which fully corresponds to the physics of the phenomenon under consideration [12, 13, 20, 21]. In this case, the previously discovered accumulation effect is observed [11, 12]. This confirms the correctness of the calculations and the accuracy of the results obtained. Incomplete agreement with experimental data indicates the need for further research. However, it should be noted that the constructed mathematical model of the phenomenon makes it possible at this stage to obtain estimates that are sufficiently acceptable for the experiment and correctly predict the 2D director dynamics of the studied processes.

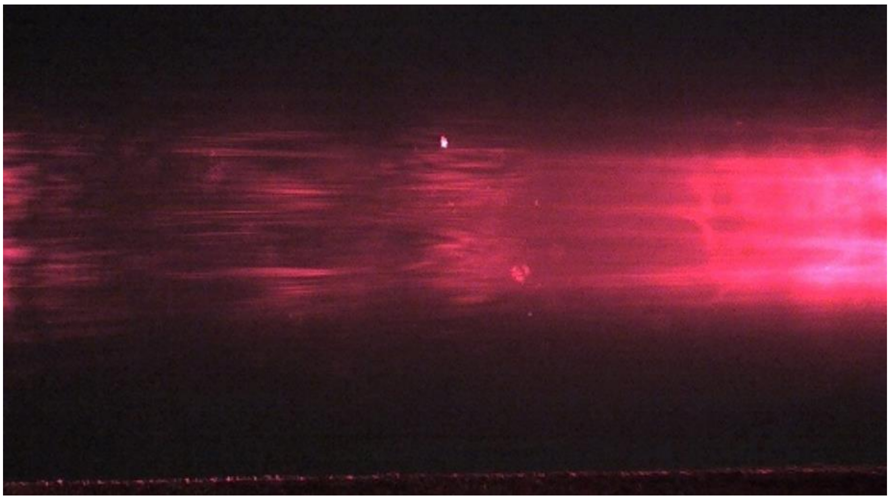
The numeric solutions for the equation and its variants (5) were obtained by the standard finite-difference methods. The programs for numerical solution and computer modeling of two-dimensional parabolic partial differential equation were developed both in FORTRAN, and C/C++ (see e.g. [12, 13, 15-18, 20-22]).

We should emphasize that this effect of the accumulation of the director deformation can affect for example the results of the SHG experiments in the nematic liquid crystal 5CB [12]. It is also important to note that the study of the effects of pulsed-periodic electric field and/or polarized laser radiation on the properties of liquid crystals and liquid-crystal waveguides undoubtedly of interest also in further research due to different possible promising applications in various applications [14, 15, 17-19, 23-25].

In the experiments, multimode irregular NLC waveguides, formed by two glass plates and LC layer between them were studied (for more details see [14, 15, 17-19, 23-25]). NLC waveguide had a homeotropic orientation of LC molecules. This work presents only some of the experimental results useful for this paper.



(*a*)



(*b*)

Fig. 4. Fragments of photo of laser radiation tracks (top view): (*a*) – quasi-TE, and (*b*) – quasi-TM-modes in one of the researched integrated optical NLC waveguide.

As one example in fig. 4 fragments of photos of the laser radiation tracks of quasi-TE and quasi-TM-modes are presented. Pulse-periodic electric field E (directed along the vertical axis of the picture) switched on.

Analyses of the laser radiation tracks in fig. 4 showed an inhomogeneous change in the attenuation coefficient α for both (quasi-TE and quasi-TM) polarizations with transverse displacement (along the x axis, see fig. 1). In neighboring mode tracks α can differ by ≈ 15–40%, and on average α is about 5–8 cm^{-1}. This indicates a fairly strong heterogeneity of the NLC layers. Under the influence of the external field E complex nonlinear processes of transformation of both the domain structures inside the layers and the characteristics of the transmitted, diffracted and scattered electromagnetic radiation were observed (see [1, 2, 7, 11-14, 17-21] for more details).

As an example, let us illustrate one case. As seen from fig. 3 in the center, the angle θ is minimal, which indicates a complete rotation of the molecules along the field (the binding energy is minimal there, in contrast to molecules at the surface of glass plates). It can be seen in fig. 4(a) that in the absence of a field E, the main part of the scattering pattern (in the center of the photo) has the character of a fairly uniform diffusion scattering by LC molecules that are almost vertically oriented (along the axis y, see fig. 1); here α ≈ 6 cm^{-1}. When the field E is switched on, the scattering pattern (especially in the center of the picture) changes, since scattering by horizontally oriented (along the axis x, see fig. 1) and tilted at an angle $\theta(x, y; t)$ (see fig. 1, fig. 2, fig. 3) molecules begins to prevail; here α ≈ 9 cm^{-1}. In this case, already more scattered radiation leaves the plane of the waveguide (coincides with the plane (x, z)) and begins to contribute to the radiation detected outside the plane of the NLC waveguide. The experimental results demonstrate a number of effects in NLC waveguides, note some of them: inhomogeneous change in modes attenuation coefficient, discrete light propagation, and self-trapping in liquid crystals (see e.g. [17, 18, 20, 21, 25-27]).

An analysis of the features of the propagation of quasi-waveguide modes shows that, in the case of dynamic processes in liquid crystal waveguides, such effects as power exchange between coupled quasi-TE and quasi-TM modes, leakage of quasi-

TE and quasi-TM modes, re-emission of incident modes into modes of a different order, etc., can be observed. Research and analysis of these effects and their possible prospective applications in different integrated optics and photonics devices is beyond the scope of this work (see for more details e.g. [17-21, 23-28]).

4. Conclusion

Different nematic liquid crystal 2D structures were researched by the numeric simulation and experimentally. The 2D dynamics of the LC director due to the external pulse-periodic electric field action was studied. The previously discovered 1D accumulation effect was confirmed by numerical modeling for the 2D case. An analysis of the features of the propagation of quasi-TE and quasi-TM modes in a liquid crystal multimode waveguide was made. A more detailed analysis of the obtained results is beyond the scope of this work since the main goal was to demonstrate the efficiency of the developed algorithms and programs for the numerical analysis of the phenomenon under study. The results obtained are important for further investigation of dynamic processes inside non-stationary liquid crystal layers, both from the theoretical point of view for understanding kinetic processes in the liquid crystals, and with practical, -- in the organization and carrying out appropriate experimental and theoretical researches in the field of the optofluidics, photonics, and waveguide optics.

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