EDN: VEGZRT
УДК 519.688

Analysis of the Unstable State of a Nematic Liquid Crystal Based on a Simplified Dynamic Model

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Received 18.05.2023, received in revised form 01.11.2023, accepted 14.02.2024

Abstract. The Fréedericksz effect consisting in the reorientation of liquid crystal molecules in an extended layer under the action of inhomogeneous electric field is simulated in the paper. The constitutive equations for tangential stress, angular velocity, and electric potential are obtained from the equations of a simplified dynamic model of a 5CB nematic liquid crystal in the acoustic approximation. The algorithm for numerical solution of the constitutive equations is constructed on the basis of finite-difference schemes. The algorithm is implemented with the use of CUDA technology for computers with graphics accelerators.

Keywords: liquid crystal, dynamics, electric potential, Fréedericksz effect, method of straight lines, Laplace equation, parallel programming, CUDA technology.

Citation: I.V. Smolekho, Analysis of the Unstable State of a Nematic Liquid Crystal Based on a Simplified Dynamic Model, J. Sib. Fed. Univ. Math. Phys., 2024, 17(3), 272–281. EDN: VEGZRT.

Introduction

Liquid crystals (LCs) have in a certain temperature range both fluidity (the property of liquids) and anisotropy (the property of solid crystals). There is an order in the spatial orientation of liquid crystal molecules which significantly affects their properties. To characterize the order a unit vector "director" is introduced. It specifies the preferred direction of the molecules. Depending on the order of orientation of molecules there are three classes of LCs: nematic (molecules are oriented in the direction of the vector-director and located randomly), smectic (molecules form layers, and each layer has its own orientation of molecules) and cholesteric (molecules are form into layers, creating a spiral). Liquid crystals are sensitive to external influences which make it possible to control their properties by changing their spatial orientation. That is why the liquid crystal state of matter is of scientific interest to researchers. Liquid crystals are widely used in creating displays of various digital devices. Due to anisotropy of the permittivity weak electric field causes the liquid crystal molecules to rotate, and it results in the change of optical properties. The reorientation of liquid crystal molecules under the action of electric field was first observed and studied by Fréedericksz and his colleagues [1]. The orientation was changed when strong enough field was applied to the liquid crystal. This effect was called the Fréedericksz transition, and it has a threshold character. Theoretically, it was studied using the elastic free energy of Frank and the energy of interaction with electric field. The Oseen–Frank model [2,

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3] describes the static state of liquid crystals. According to the theory, the field causes such deformation of the liquid crystal that distribution of molecules corresponds to minimum of the free energy which is equal to the sum of elastic and dielectric components. The elastic energy is a quadratic form in terms of derivatives of the vector-director with respect to spatial coordinates. However, this model cannot be generalized for the analysis of dynamic processes. It does not take into account translational motion because only rotational motion is considered. By now universal dynamic model has been developed by Eriksen [4] and Leslie [5]. It is based on conservation laws and takes into account translational and rotational degrees of freedom of molecules. This theory describes the flow of nematic liquid crystal from the hydrodynamic point of view, and it is reduced to the Oseen–Frank theory in the static case. The need to create new dynamic models of liquid crystal is dictated by the complexity of the existing universal Eriksen–Leslie model that requires construction of state functions using specific experiments. A simplified dynamic model in the acoustic approximation was proposed [6]. It includes equations of acoustics and heat conduction. These equations are based on conservation laws and the Cosserat continuum model, and they include small independent rotations of particles in addition to translational motion. The model describes he dynamic behaviour of nematic liquid crystals under the action of mechanical, thermal and electrical external factors.

Analysis of an unstable state in statics was carried out in [7], where the governing equations of the model are non-linear variational Euler equations for the electric potential and the orientation angle of molecules in the problem of minimizing the potential energy functional.

This work is devoted to modelling the reorientation of molecules in an extended liquid crystal layer located in the electric field of a capacitor with short plates arranged periodically. The governing equations are obtained from the simplified dynamic model of the liquid crystal in the acoustic approximation. The developed parallel numerical algorithm is based on an explicit difference scheme of the second order of approximation. The accuracy of numerical solution can be improved by choosing a finer grid due to the distribution of computational load. The computational algorithm is implemented as a software package written in C++ by means of CUDA technology using video card graphics accelerators.

1. Formulation of the problem

The governing partial differential equations for the angular velocity ω and tangential stress q are obtained by differentiating the equations of the simplified dynamic model of the nematic liquid crystal:

$$\begin{gathered}\frac{\partial^2 q}{\partial t^2}+\frac{2\,\alpha}{\eta}\,\frac{\partial q}{\partial t}+2\,\alpha\,\frac{\partial \omega}{\partial t}=\frac{\alpha}{\rho}\left(\triangle q+\frac{\partial f_2}{\partial x_1}-\frac{\partial f_1}{\partial x_2}\right),\\ \frac{\partial^2 \omega}{\partial t^2}-\frac{2}{j}\,\frac{\partial q}{\partial t}=\frac{\gamma}{j}\,\triangle\omega+\frac{1}{j}\,\frac{\partial m}{\partial t}.\end{gathered}\tag{1}$$

Here ρ is the density, j is the moment of inertia, η is the viscosity coefficient, α is the modulus of elastic resistance to rotation, γ is the modulus of elastic resistance to curvature change. Equations (1) describe moment interactions of liquid crystal molecules under the action of inhomogeneous electric field in a two-dimensional formulation. This model of the effect of the Fréedericksz reorientation have a fewer number of equations in comparison with the general model. The initial data for q and ω are

$$q\Big|_{t=0} = q^0, \quad \omega\Big|_{t=0} = \omega^0, \quad \frac{\partial q}{\partial t}\Big|_{t=0} = -2\,\alpha\Big(\omega^0 + \frac{q^0}{\eta}\Big), \quad \frac{\partial \omega}{\partial t}\Big|_{t=0} = \frac{2\,q^0 + m}{j},$$

where q^0, ω^0 are the values of the required quantities at the initial moment of time. The initial linear velocities and moment stresses are assumed to be equal to zero. The boundary conditions are formulated in terms of q and ω. The symmetry conditions for stress state of the liquid crystal are given in terms of derivatives q_{x_1}, ω_{x_1} or q_{x_2}, ω_{x_2} (depending on the symmetry line).

During the action of electric field bulk forces $f = (P \cdot \nabla)\, E$ and moment of forces $m = P \times E$ arise. Here $E = -\nabla\varphi$ is the electric field vector, $P = \varepsilon_0\, \chi\, E$ is the electric polarization vector, $\chi = \varepsilon - I$ is the dielectric susceptibility tensor, and ε is the dielectric susceptibility tensor. In a 2D formulation of the problem bulk forces and moment of forces are defined as follows

$$\begin{aligned} f_1 &= \varepsilon_0\Big(\chi_{11}\,\frac{\partial\varphi}{\partial x_1} + \chi_{12}\,\frac{\partial\varphi}{\partial x_2}\Big)\frac{\partial^2\varphi}{\partial x_1^2} + \varepsilon_0\Big(\chi_{12}\,\frac{\partial\varphi}{\partial x_1} + \chi_{22}\,\frac{\partial\varphi}{\partial x_2}\Big)\frac{\partial^2\varphi}{\partial x_1 \partial x_2}, \\ f_2 &= \varepsilon_0\Big(\chi_{11}\,\frac{\partial\varphi}{\partial x_1} + \chi_{12}\,\frac{\partial\varphi}{\partial x_2}\Big)\frac{\partial^2\varphi}{\partial x_1 \partial x_2} + \varepsilon_0\Big(\chi_{12}\,\frac{\partial\varphi}{\partial x_1} + \chi_{22}\,\frac{\partial\varphi}{\partial x_2}\Big)\frac{\partial^2\varphi}{\partial x_2^2}, \\ m &= \varepsilon_0\,(\chi_{11} - \chi_{22})\,\frac{\partial\varphi}{\partial x_1}\,\frac{\partial\varphi}{\partial x_2} - \varepsilon_0\,\chi_{12}\Big(\Big(\frac{\partial\varphi}{\partial x_1}\Big)^2 - \Big(\frac{\partial\varphi}{\partial x_2}\Big)^2\Big). \end{aligned} \tag{2}$$

The permittivity along molecules$\varepsilon_{\|}$ and permittivity across molecules $\varepsilon_{\perp}$ are different. Components of ε tensor depend on rotation angle of molecules θ:

$$\varepsilon_{11} = \varepsilon_{\|}\cos^2\theta + \varepsilon_{\perp}\sin^2\theta, \quad \varepsilon_{22} = \varepsilon_{\|}\sin^2\theta + \varepsilon_{\perp}\cos^2\theta, \quad \varepsilon_{12} = \varepsilon_{21} = \big(\varepsilon_{\|} - \varepsilon_{\perp}\big)\cos\theta\sin\theta,$$

Relations for calculating components of the permittivity tensor contain rotation angle that changes each time step when solving dynamic problem. Thus, it is necessary to add an equation for the rotation angle to system of equations (1):

$$\frac{\partial\theta}{\partial t} = \omega. \tag{3}$$

Bulk forces and moment of forces (2) are taken into account in the right parts of governing equations (1). In turn, a change in the spatial orientation of molecular domains due to the action of forces and moment of forces leads to a change in the permittivity tensor. Then, electric field is changed.

The perturbation by the electric field occurs as follows. A horizontally infinite flat liquid crystal layer located between short capacitor plates is considered. Potential difference is set between upper and bottom plates: $\varphi^+ = \varphi^0$, $\varphi^- = -\varphi^0$. Conditions for the continuity of the electric potential (between the dielectric and air) and the continuity of the normal component of the electric induction vector are set at the interface:

$$\begin{aligned} &\varphi^+ = \varphi, \quad \frac{\partial\varphi^+}{\partial x_2} = \varepsilon_{12}\,\frac{\partial\varphi}{\partial x_1} + \varepsilon_{22}\,\frac{\partial\varphi}{\partial x_2} \quad \text{if} \;\; x_2 = h, \\ &\varphi = \varphi^-, \quad \varepsilon_{12}\,\frac{\partial\varphi}{\partial x_1} + \varepsilon_{22}\,\frac{\partial\varphi}{\partial x_2} = \frac{\partial\varphi^-}{\partial x_2} \quad \text{if} \;\; x_2 = 0. \end{aligned}$$

The initial distribution of orientation angles θ_0 relative to the x_1 axis is known inside the layer. It is given, for example, as shown in Fig. 1. Angle θ is calculated in succeeding time steps using the difference analogue of equation (3).

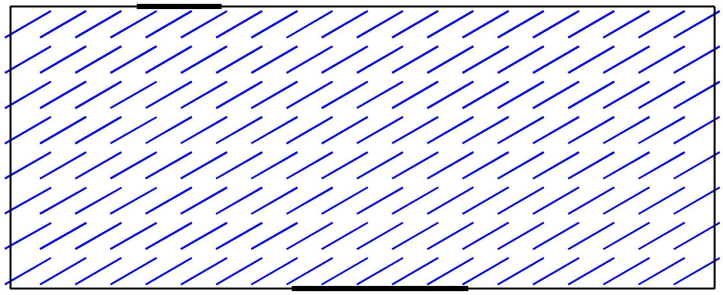

Fig. 1. Scheme of perturbation of the liquid crystal layer by an electric field

2. Computational algorithm

The solution of the problem includes several stages. At the first stage, it is necessary to calculate the values of the electric potential included in (2). The electric potential satisfies the anisotropic equation $\nabla \cdot (\varepsilon \cdot \nabla\varphi) = 0$ in the LC layer. To solve this equation the finite difference method is used to implement an iterative process in which the Poisson equation is recursively solved using fast Fourier transform with respect to new approximation of the potential φ^{n+1}:

$$\tilde{\varepsilon}\,\triangle\varphi^{n+1} = \tilde{\varepsilon}\,\triangle\varphi^{n} - \nabla \cdot (\varepsilon \cdot \nabla\varphi^{n}).$$

Here the right hand side is calculated using approximation from the previous time step φ^n, constant $\tilde{\varepsilon}$ is chosen in such a way that iterative process converges. The process continues until the relative error defined as the uniform difference norm becomes sufficiently small. Calculations showed that no more than 10 iterations are required for the convergence of the iterative process with a relative error of 10^{-5} for $\tilde{\varepsilon} = (\varepsilon_{\parallel} + \varepsilon_{\perp})/2$.

The Laplace equation $\Delta\varphi = 0$ is satisfied outside the LC layer. It is solved by the method of straight lines. The segment is uniformly partitioned in the direction x_1, and derivatives with respect to x_2 are replaced by finite differences. Thus, function φ is discrete in the direction x_1 and continuous in the direction x_2. Further, the solution is constructed using the Fourier transform. To calculate the solution, the same rectangular grid is considered for both solutions. The algorithm of calculation of electrical action on the liquid crystal layer is described in detail in [8]. After finding the values of the electric potential, bulk forces and moment of forces are calculated using (2) where partial derivatives are replaced with finite differences. At the last stage, using the explicit second order of accuracy finite-difference scheme "cross" values of q and ω are determined:

$$\omega_{i_1,i_2}^{n+1} = 2\,\omega_{i_1,i_2}^{n} - \omega_{i_1,i_2}^{n-1} + \frac{\triangle t}{j}\Big(q_{i_1,i_2}^{n+1} - q_{i_1,i_2}^{n-1}\Big) +$$
$$+ \frac{\gamma\,(\triangle t)^2}{j}\left(\frac{\omega_{i_1+1,i_2}^{n} - 2\,\omega_{i_1,i_2}^{n} + \omega_{i_1-1,i_2}^{n}}{(\triangle x_1)^2} + \frac{\omega_{i_1,i_2+1}^{n} - 2\,\omega_{i_1,i_2}^{n} + \omega_{i_1,i_2-1}^{n}}{(\triangle x_2)^2}\right) + \qquad (4)$$
$$+ \frac{\triangle t}{2\,j}\Big(m_{i_1,i_2}^{n} - m_{i_1,i_2}^{n-1}\Big),$$

$$\left(\frac{\alpha}{j}+\frac{\alpha}{\eta\,\triangle t}+\frac{1}{(\triangle t)^2}\right)q^{n+1}_{i_1,i_2}=\frac{2}{(\triangle t)^2}\,q^{n}_{i_1,i_2}+\frac{2\,\alpha}{\triangle t}\Big(\omega^{n-1}_{i_1,i_2}-\omega^{n}_{i_1,i_2}\Big)+$$
$$+\left(\frac{\alpha}{j}+\frac{\alpha}{\eta\,\triangle t}-\frac{1}{(\triangle t)^2}\right)q^{n-1}_{i_1,i_2}+\frac{\alpha}{\rho}\Bigg(\frac{q^{n}_{i_1+1,i_2}-2\,q^{n}_{i_1,i_2}+q^{n}_{i_1-1,i_2}}{(\triangle x_1)^2}+$$
$$+\frac{q^{n}_{i_1,i_2+1}-2\,q^{n}_{i_1,i_2}+q^{n}_{i_1,i_2-1}}{(\triangle x_2)^2}+\frac{f_2{}^{n}_{i_1+1,i_2}-f_2{}^{n}_{i_1-1,i_2}}{2\,\triangle x_1}- \tag{5}$$
$$-\frac{f_1{}^{n}_{i_1,i_2+1}-f_1{}^{n}_{i_1,i_2-1}}{2\,\triangle x_2}\Bigg)+\frac{\alpha}{2\,j}\Big(m^{n}_{i_1,i_2}-m^{n-1}_{i_1,i_2}\Big)-$$
$$-\frac{\alpha\,\gamma\,\triangle t}{j}\left(\frac{\omega^{n}_{i_1+1,i_2}-2\,\omega^{n}_{i_1,i_2}+\omega^{n}_{i_1-1,i_2}}{(\triangle x_1)^2}+\frac{\omega^{n}_{i_1,i_2+1}-2\,\omega^{n}_{i_1,i_2}+\omega^{n}_{i_1,i_2-1}}{(\triangle x_2)^2}\right).$$

Then rotation angle is recalculated as follows

$$\theta^{n+1}_{i_1,i_2}=\theta^{n}_{i_1,i_2}+\frac{\Delta t}{2}\Big(\omega^{n+1}_{i_1,i_2}+\omega^{n}_{i_1,i_2}\Big).$$

3. Analysis of the unstable state of LC based on the Oseen–Frank model

When the potential difference is below of some threshold value, an oscillatory motion of molecules occurs with a small deviation from the initial position. The static Oseen–Frank theory is used to estimate the instability of the equilibrium of the liquid crystal. In accordance with the theory, the distribution of orientation angles of molecules in the equilibrium state of the LC layer under the action of electric field created by charges on the plates satisfies the stationarity condition for the potential energy functional:

$$J=\int_V\Big(F-\frac{1}{2}\,D\cdot E\Big)\,dV\,.$$

Here V is the rectangular area selected in accordance with the symmetry of the problem, $E=$ $=-\big(0,\varphi_{x_2},0\big)$, $D=\varepsilon_0\,\varepsilon_{\,\perp}\,E+\varepsilon_0\,\Delta\varepsilon\,(n\cdot E)\,n$, $\Delta\varepsilon=\varepsilon_{\,\parallel}-\varepsilon_{\,\perp}$. The Frank free energy F in the one-constant approximation takes the form

$$F=\frac{1}{2}\,\gamma\Big(|\nabla\cdot n|^2+|\nabla\times n|^2\Big). \tag{6}$$

The vector-director responsible for the predominant direction of liquid crystal molecules depends in this case only on x_2: $n=\big(\cos\theta(x_2),\sin\theta(x_2),0\big)$. The equilibrium of liquid crystal molecules is achieved by minimizing the Oseen–Frank free energy functional:

$$\int_V\Big(F-\frac{1}{2}\,D\cdot E\Big)\,dV\;\to\;\min, \tag{7}$$

where

$$D\cdot E=\varepsilon_0\,\varepsilon_{\,\perp}E^2+\varepsilon_0\,\Delta\varepsilon\,(n\cdot E)^2. \tag{8}$$

Taking into account that the first term in expression (8) does not depend on n and n in turn does not depend on x_1, this expression takes the form

$$D\cdot E=\varepsilon_0\,\varepsilon_{\,\perp}\left(\frac{d\varphi}{dx_2}\right)^2+\;\varepsilon_0\,\Delta\varepsilon\left(\frac{d\varphi}{dx_2}\right)^2\sin^2\theta.$$

After substituting (6) and (8) into (7) and taking into account that $\sin\theta \approx \theta$, one can obtain

$$\int_0^h \left[\frac{\gamma}{2}\left(\frac{d\theta}{dx_2}\right)^2 - \frac{1}{2}\,\varepsilon_0\,\varepsilon_\perp\left(\frac{d\varphi}{dx_2}\right)^2 - \frac{1}{2}\,\varepsilon_0\,\Delta\varepsilon\left(\frac{d\varphi}{dx_2}\right)^2\theta^2\right]dx_2 \;\to\; \min.$$

Varying the functional and integrating it by parts, one can obtain that

$$\int_0^h \left[-\gamma\,\frac{d^2\theta}{dx_2^2} - \varepsilon_0\,\Delta\varepsilon\left(\frac{d\varphi}{dx_2}\right)^2\theta\right]\delta\theta\;dx_2 = 0.$$

Thus, the Euler equation is obtained:

$$\gamma\,\frac{d^2\theta}{dx_2^2} = -\,\varepsilon_0\,\Delta\varepsilon\left(\frac{d\varphi}{dx_2}\right)^2\theta. \tag{9}$$

The following chain of transformations is valid

$$\theta = e^{\lambda x_2}, \quad \gamma\,\lambda^2 = -\,\varepsilon_0\,\Delta\varepsilon\left(\frac{d\varphi}{dx_2}\right)^2, \quad \lambda = \pm\,i\sqrt{\frac{\varepsilon_0\,\Delta\varepsilon\left(\frac{d\varphi}{dx_2}\right)^2}{\gamma}};$$

$$\theta = \sin\sqrt{\frac{\varepsilon_0\,\Delta\varepsilon\left(\frac{d\varphi}{dx_2}\right)^2}{\gamma}}\;x_2\Big|_0^h = 0 \quad\Rightarrow\quad \sqrt{\frac{\varepsilon_0\,\Delta\varepsilon\left(\frac{d\varphi}{dx_2}\right)^2}{\gamma}}\;h = \pi.$$

Minimization of the functional gives an estimate of the instability at which the functional loses its convexity. Corresponding Euler equation (9) with boundary conditions $\theta(0) = \theta(h) = 0$ has non-trivial solutions

$$\varphi^+ - \varphi^- = \pi\sqrt{\frac{\gamma}{\varepsilon_0\,\Delta\varepsilon}}.$$

For a 5CB liquid crystal with $\gamma = 6\cdot 10^{-12}$ H, $\varepsilon_\parallel = 16.7$, $\varepsilon_\perp = 7$ the threshold value the potential difference is about 1 V. Above this value, the molecules lose their stability and turn along the direction of the field, forming swarms of identically oriented molecules.

4. Calculation results

A parallel program implementing the described algorithms is written in C++ using CUDA technology for computing systems with graphics accelerators. The calculations were carried out on the high-performance Flagman server of ICM SB RAS.

In all calculations, the coefficients for the 5CB liquid crystal were taken according to experimental data [9]. Earlier, the value of coefficient $\alpha = \nu^2 j\,\pi^2$ was based on the resonant frequency $\nu^* = 350$ MHz obtained experimentally in [10]. In the present work, calculations were carried out for various values of ν. It was studied how the orientation of molecules changes at different time steps in this case. The bulk density of the moment of inertia is determined as $j = \rho\,(N\delta_0)^2/12$, where $\delta_0 = 1.87$ nm, $N = 10$, $\rho = 1022$ kg/m^3. A finite difference grid is introduced in the space x_1, x_2 with the space step Δx_1 in the direction x_1 and the space step Δx_2 in the direction x_2. The time step is defined as Δt. The grid consists of a set of nodes $R^n_{i_1,i_2} = R(t_n, x_{1i_1}, x_{2i_2})$. Loads can be specified on some sections of the boundary.

Figs. 2–4 show the results of calculations for $10 \times 4\,\mu$m liquid crystal layer under the action of electric field for various initial orientations of molecules and various arrangements of plates.

The horizontal lines show the boundaries of the layer exposed to electric field. The thick lines show the capacitor plates. The capacitor plates are arranged non-symmetrically in Fig. 2 *a*, and they are arranged symmetrically in Fig. 2 *b*. The length of the upper plate is 1 μm, the length of the lower plate is 2.5 μm in both calculations. The finite difference grid in the LC layer contains 640×256 cells, and in the outer parts of the layer it contains 640×128 cells.

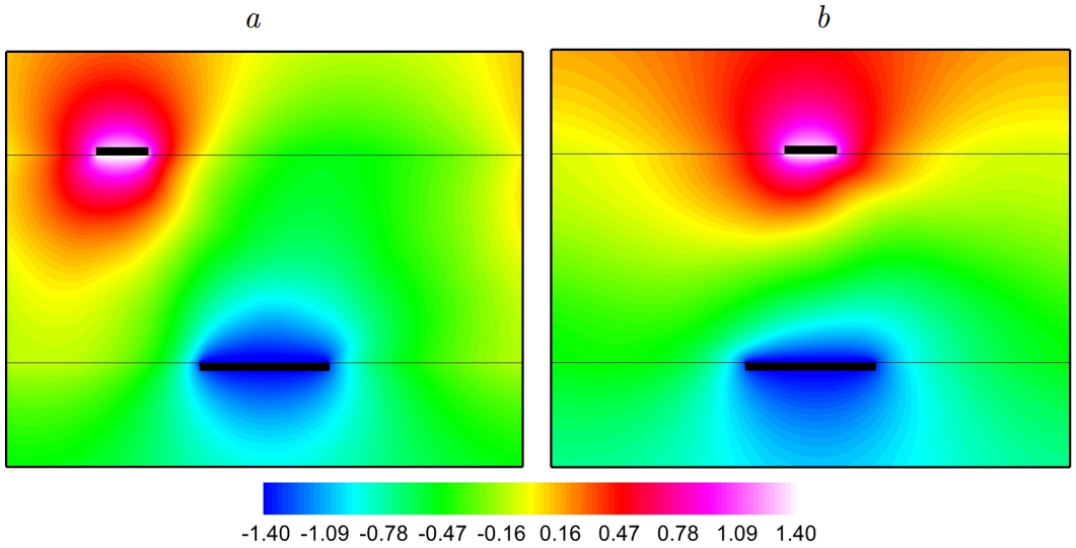

Fig. 2. Disturbance of the LC layer by electric field: level lines of electric potential φ at 10000th time step; rotation angle of molecules $\theta = \pi/4$ (*a*), 0 (*b*)

Fig. 3 shows the level lines for the rotation angle of molecules in the LC layer for the problem in Fig. 2 *a* for different α and ν at various time steps. The results for $\nu = 11$ MHz and $\alpha = 0.36$ Pa are shown on the left side, and results for $\nu = 35$ MHz and $\alpha = 3.6$ Pa are shown on the right side. The potential difference is 1.5 V that exceeds the threshold value of 1 V. Therefore, liquid crystal molecules are reoriented in the direction of the electric field. One can also observe the effect of formation of large domains of identically oriented molecules (so-called swarms), the size of which changes with time.

Fig. 4 shows level lines with similar parameters but for symmetrical capacitor plates for the problem in Fig. 2 *b*.

It is noted that the smaller ν and hence coefficient α the larger swarms are formed which more slowly break up into smaller ones over time. Swarms disintegrate already at 20000 – 25000 time step for $\nu = 35$ MHz. That is not observed for $\nu = 11$ MHz.

Conclusion

This paper presents mathematical model of the action of electrical field on liquid crystals. Equations of the model are obtained from the previously developed dynamic model within the framework of acoustic approximation. The model allows one to significantly speed up the time of calculations. The algorithm for numerical solution of model equations is implemented as a parallel program in C++ using CUDA technology.

The developed model can be used to study the behaviour of liquid crystals under the action of electric field in dynamics and formation of swarms depending on the intensity of electric field, the

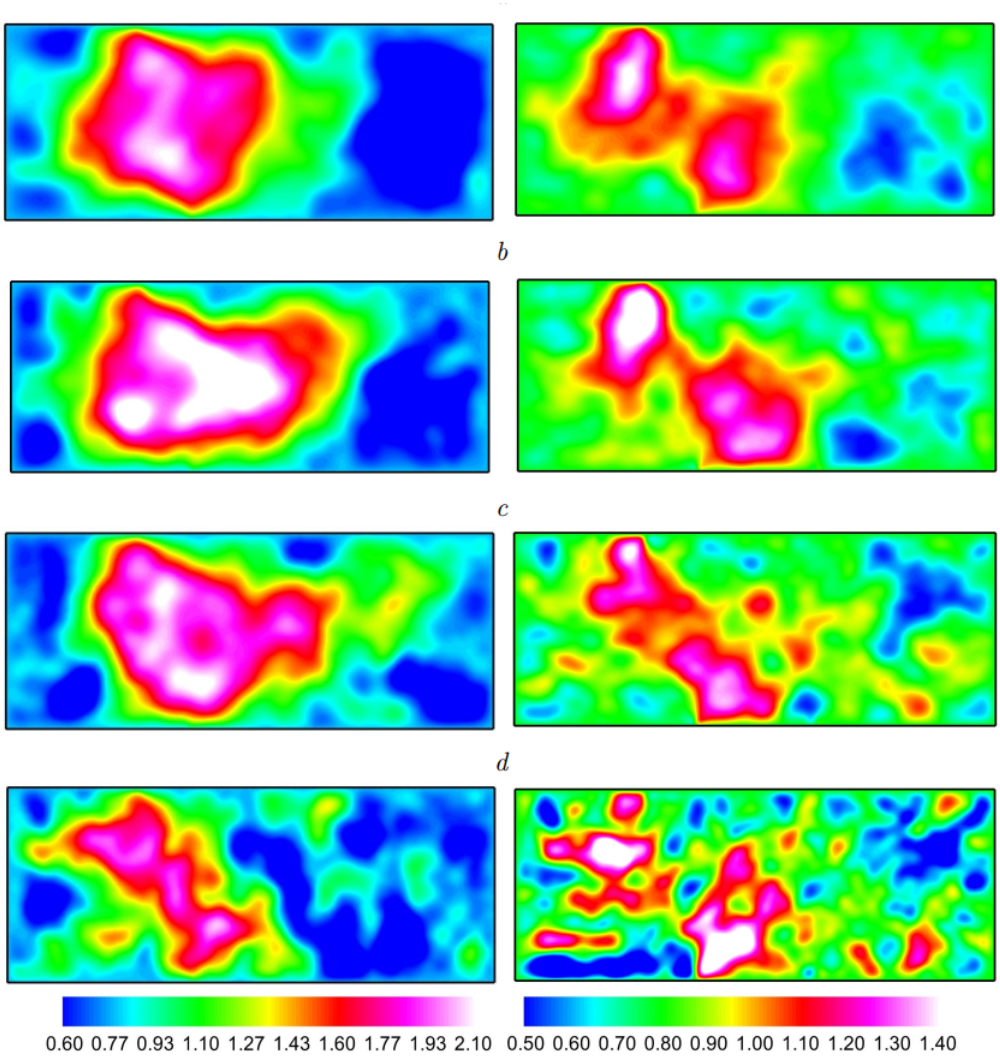

Fig. 3. Distribution of orientation angles of LC molecule domains with symmetrical arrangement of plates: 5000th (a), 10000th (b), 15000th (c), 25000th (d) time steps

initial rotation angle of molecules and location of the capacitor plates. The results showed that as frequency increases smaller swarms are formed which quickly break up into smaller swarms. The results of calculations can be applied to the study of the dynamics of liquid crystals in the problems of propagation of thermoelastic waves caused by weak mechanical and electrical disturbances.

This work is supported by the Krasnoyarsk Mathematical Center and financed by the Ministry of Science and Higher Education of the Russian Federation in the framework of the establishment and development of regional Centers for Mathematics Research and Education (Agreement No. 075-02-2023-912).

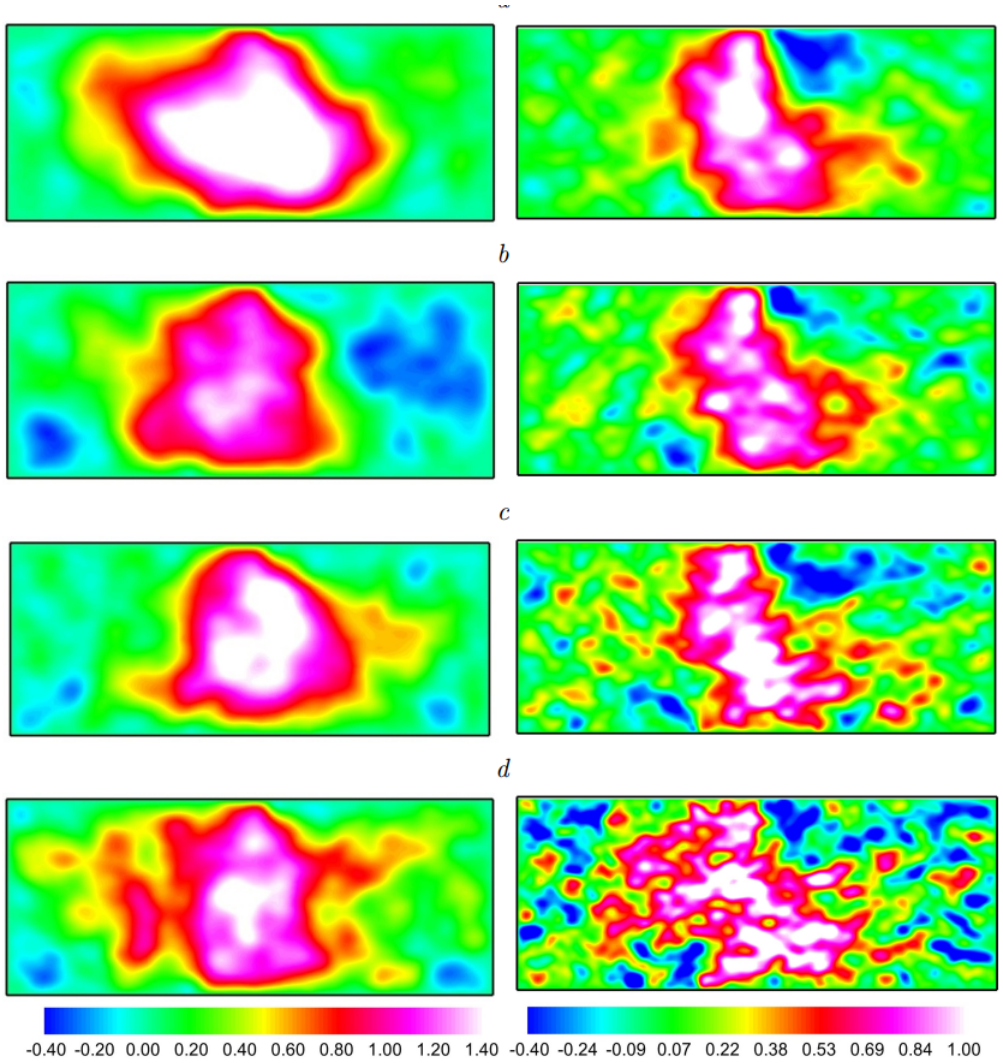

Fig. 4. Distribution of orientation angles of LC molecule domains with symmetrical arrangement of plates: 5000th (a), 10000th (b), 15000th (c), 25000th (d) time steps

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Анализ неустойчивого состояния нематического жидкого кристалла на основе упрощенной динамической модели

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Аннотация. В статье моделируется эффект Фредерикса, состоящий в переориенации молекул жидкого кристалла в протяженном слое под действием неоднородного электрического поля. Определяющие уравнения для касательного напряжения, угловой скорости и электрического потенциала получены из уравнений упрощенной динамической модели нематического жидкого кристалла 5ЦБ в акустическом приближении. Построен алгоритм численного решения определяющих уравнений с помощью конечно-разностных схем. Программная реализация алгоритма выполнена по технологии CUDA для компьютеров с графическими ускорителями.

Ключевые слова: жидкий кристалл, динамика, электрический потенциал, эффект Фредерикса, метод прямых, уравнение Лапласа, параллельное программирование, технология CUDA.