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Investigation of the Orientational Thermoelasticity Effect Using a Simplified Model of Nematic Liquid Crystal in the Acoustic Approximation

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Abstract. Analysis of the orientational thermoelasticity effect using a two-dimensional simplified dynamic model of liquid crystal in the acoustic approximation is presented in the paper. It is assumed that effect occurs when one of the boundaries of a rectangular liquid crystal layer is heated. To solve the system of model equations, the method of two-cycle splitting with respect to spatial variables is used in combination with the finite-difference Godunov scheme for the acoustic equations and the Ivanov scheme with controlled energy dissipation for the heat conduction equation. This combination of finite-difference methods allows one to calculate related thermomechanical processes using the same time and space steps that satisfy the Courant-Friedrichs-Levy criterion. The numerical algorithm was implemented as a parallel program written in C++. Parallelization of computations was performed with NVIDIA graphic accelerators using CUDA technology. Simulations demonstrate that it is impossible to observe the effect of reorientation of liquid crystal molecules under the influence of temperature for the presented simplified model in the acoustic approximation. It was concluded that when surface tension forces are taken into account this effect will be observed for the model used in this work.

Keywords: liquid crystal, thermal conductivity, dynamics, CUDA technology.

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Introduction

Liquid crystals are substances combining the optical anisotropy of crystals and the molecular mobility of liquids in some temperature range. This is the most important property of such systems [1, 2]. Liquid crystal molecules have a specific shape but they also have the property of fluidity. Depending on the initial orientation, liquid crystals are divided into nematic, smectic and cholesteric. The most common type of liquid crystals, namely, nematic crystal is considered in present which best reflects the dual nature of these substances. This type has a wide range of applications, ranging from information display technologies to optical devices and sensors. It helps to regulate the brightness of the screen in LCDs by changing the strength of the electric field acting on the crystal. In addition, orientation of liquid crystals is sensitive to temperature change. If liquid crystals are heated they take a more ordered state which can be used, for example, for data storage. If such liquid crystals are cooled they return to their original state. It means that data can be erased and rewritten. Liquid crystal sensors are used for temperature

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measurement and biochemical analysis, they continue to be of interest due to their controllable optical and electro-optical properties. Studies in this field are progressing, and new applications are being developed so liquid crystals play an important role in modern constantly evolving technologies. By now, dynamic model of Ericksen and Leslie [3, 4] has been developed on the basis of conservation laws. It takes into account all types of movements as well as the flow of liquid crystals. However, it turned out to be too complex to solve using numerical methods because it includes a large number of equations and parameters that must be determined experimentally which is not always possible. Then, there was a need to develop simpler models allowing for a detailed description of the processes occurring in liquid crystals that would significantly facilitate their study.

This paper presents analysis of the orientational thermoelasticity effect using a simplified two-dimensional model in the acoustic approximation. It takes into account mechanical, temperature and electrical effects in liquid crystals [5]. The effect occurs when the boundary of a horizontal liquid crystal layer is heated. The effect of temperature on the orientation of liquid crystal molecules was studied experimentally [6]. It was concluded that susceptibility to heat flows is similar to the interaction with electromagnetic fields. However, a plate with significantly different coefficient of volumetric expansion was used in experiments. It is likely that the effect of molecular reorientation is associated with the thermal expansion of the plate but not with the effect of the heat flow.

1. Mathematical model of liquid crystal in acoustic approximation

The equations of the model that describe behaviour of liquid crystals under thermomechanical and electrical perturbations are derived from the integral conservation laws of energy, momentum, and angular momentum on the basis of the Cosserat continuum theory [7] using the Clausius–Duhem inequality. In the planar case, the model includes the following equations

translational motion
$$\rho\,\frac{\partial v_1}{\partial t} = -\frac{\partial p}{\partial x_1} - \frac{\partial q}{\partial x_2} + f_1, \quad \rho\,\frac{\partial v_2}{\partial t} = \frac{\partial q}{\partial x_1} - \frac{\partial p}{\partial x_2} + f_2, \tag{1}$$

rotational motion
$$J\,\frac{\partial \omega}{\partial t} = 2\,q + \frac{\partial \mu_1}{\partial x_1} + \frac{\partial \mu_2}{\partial x_2} + m, \tag{2}$$

couple stresses
$$\frac{\partial \mu_1}{\partial t} = \gamma\,\frac{\partial \omega}{\partial x_1}, \quad \frac{\partial \mu_2}{\partial t} = \gamma\,\frac{\partial \omega}{\partial x_2}, \tag{3}$$

angle of rotation
$$\frac{\partial \theta}{\partial t} = \omega, \tag{4}$$

state for pressure and tangential stress
$$\frac{\partial p}{\partial t} = -\kappa\left(\frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2}\right) + \beta\,\frac{\partial T}{\partial t}, \quad \frac{\partial q}{\partial t} = \alpha\left(\frac{\partial v_2}{\partial x_1} - \frac{\partial v_1}{\partial x_2}\right) - 2\,\alpha\left(\omega + \frac{q}{\eta}\right), \tag{5}$$

anisotropic heat conduction
$$\rho\, c\,\frac{\partial T}{\partial t} = \frac{\partial}{\partial x_1}\left(æ_{11}\,\frac{\partial T}{\partial x_1} + æ_{12}\,\frac{\partial T}{\partial x_2}\right) + \frac{\partial}{\partial x_2}\left(æ_{12}\,\frac{\partial T}{\partial x_1} + æ_{22}\,\frac{\partial T}{\partial x_2}\right) - \tag{6}$$

$$-\beta T\left(\frac{\partial v_1}{\partial x_1}+\frac{\partial v_2}{\partial x_2}\right)+\frac{2\,q^2}{\eta}+H,$$

$$æ_{11}=æ_{\|}\cos^2\theta\;+æ_{\perp}\sin^2\theta,\qquad æ_{12}=(æ_{\|}-æ_{\perp})\sin\theta\cos\theta,\qquad æ_{22}=æ_{\|}\sin^2\theta+æ_{\perp}\cos^2\theta,$$

where v_1 and v_2 are the components of the velocity vector, ω is the angular velocity, θ is the rotation angle of molecules, p is the pressure, q is the tangential stress, μ_1 and μ_2 are the couple stresses, T is the temperature, ρ is the density, J is the moment of inertia, κ is the bulk compression modulus, α is the modulus of elastic resistance to rotation, β is the coefficient of thermal expansion, γ is the modulus of elastic resistance to curvature change, η is the viscosity coefficient, H is the intensity of heat sources, c is the specific heat capacity, $æ_{\|}$ and $æ_{\perp}$ are the thermal conductivity coefficients of a liquid crystal in the direction of molecular orientation and in the transverse direction, f_1, f_2 and m are the bulk forces and couple force caused by the electric field. Here, they are not taken into account when studying the thermodynamic effect since they do not affect the temperature change. The algorithm of the electric effect is presented, for example, in [8].

2. Computational algorithm

A rectangular region of liquid crystal is considered with dimensions lx_1 and lx_2 in the directions x_1 and x_2, respectively. The finite-difference grid is

$$R^i_{i_1\,i_2}=\{(t_i,x_{1_{i_1}},x_{2_{i_2}}):t_i=i\,\Delta t,\quad x_{1_{i_1}}=i_1\Delta x_1,\quad x_{2_{i_2}}=i_2\Delta x_2,$$
$$i=0,\dots,Nt,\quad i_1=0,\dots,Nx_1,\quad i_2=0,\dots,Nx_2\},$$

where Δx_1 and Δx_2 are space steps in the directions x_1 and x_2 such that $x_{1_{i_1}}\in(0,l_{x_1})$, $x_{2_{i_2}}\in(0,l_{x_2})$, Δt is the time step, Nt is the number of time steps, Nx_1 and Nx_2 are the arbitrary numbers of cells of the finite difference grid in the directions x_1 and x_2. At the initial moment of time, zero values are set in this region for all quantities except $\theta=\theta_0$ and $T=T_0$. The boundary conditions are presented in terms of pressure, velocity, stress and temperature. The load on the boundary can act continuously or for a given number of time steps.

System of equations (1)–(6) is hyperbolic in the sense of Friedrichs so the formulation of the Cauchy problem is correct. The system is solved using the method of two-cycle splitting by spatial variables, and it is assumed that five consecutive stages occur at each time step. At the 1st and 5th stages, one-dimensional equations that depend on x_1 are solved at different half-steps in time:

$$\left\{\begin{aligned}&\rho\,\frac{\partial v_1}{\partial t}=-\,\frac{\partial p}{\partial x_1}\\&\frac{\partial p}{\partial t}=-\,\kappa\,\frac{\partial v_1}{\partial x_1}\end{aligned}\right.,\qquad\left\{\begin{aligned}&\rho\,\frac{\partial v_2}{\partial t}=\frac{\partial q}{\partial x_1}\\&\frac{\partial q}{\partial t}=\alpha\,\frac{\partial v_2}{\partial x_1}\end{aligned}\right.,\qquad\left\{\begin{aligned}&J\,\frac{\partial \omega}{\partial t}=\frac{\partial \mu_1}{\partial x_1}\\&\frac{\partial \mu_1}{\partial t}=\gamma\,\frac{\partial \omega}{\partial x_1}\end{aligned}\right.,\tag{7}$$

$$\rho\,c\,\frac{\partial T}{\partial t}=\frac{\partial h_1}{\partial x_1}-\beta\,T\,\frac{\partial v_1}{\partial x_1},\quad h_1=æ_{11}\,\frac{\partial T}{\partial x_1}+æ_{12}\,\frac{\partial T}{\partial x_2}.\tag{8}$$

To solve equations (7), the finite-difference Godunov scheme [9] of the "predictor-corrector" type is used. At the "predictor" step, the following equations on characteristics obtained from

(7) are used

$$\begin{aligned} dx_1 &= \mp\sqrt{\kappa/\rho}\,dt: \quad dI_1^{\pm}=0, \quad I_1^{\pm} = p \pm v_1\sqrt{\kappa\rho} \\ dx_1 &= \pm\sqrt{\alpha/\rho}\,dt: \quad dI_2^{\pm}=0, \quad I_2^{\pm} = q \pm v_2\sqrt{\alpha\rho} \\ dx_1 &= \pm\sqrt{\gamma/J}\,dt: \quad dI_3^{\pm}=0, \quad I_3^{\pm} = \mu_1 \pm \omega\sqrt{\gamma J}. \end{aligned} \tag{9}$$

These equations allow one to determine the values with fractional indices on the lateral faces of the cells of the finite difference grid in the plane x_1 and t:

$$\begin{aligned} &v_{1_{i_1-1/2}} = \frac{I^+_{1,i_1-1} - I^-_{1,i_1}}{2\sqrt{\rho\kappa}}, \quad p_{i_1-1/2} = \frac{I^+_{1,i_1-1} + I^-_{1,i_1}}{2}, \quad v_{2_{i_1-1/2}} = \frac{I^+_{2,i_1} - I^-_{2,i_1-1}}{2\sqrt{\rho\alpha}}, \\ &q_{i_1-1/2} = \frac{I^+_{2,i_1} + I^-_{2,i_1-1}}{2}, \quad \omega_{i_1-1/2} = \frac{I^+_{3,i_1} - I^-_{3,i_1-1}}{2\sqrt{\gamma J}}, \quad \mu_{1_{i_1-1/2}} = \frac{I^+_{3,i_1} + I^-_{3,i_1-1}}{2}, \end{aligned} \tag{10}$$

where integer indices refer to the internal nodes of the grid $i_1 = 2,\dots,Nx_1$. At the boundary nodes, these values are found from the boundary conditions. Then heat conduction equation (7) is solved with the help of the Ivanov finite-difference scheme [10] that is used to solve problems of the dynamics of solids, plates and shells. The idea of the method is to implement the law of conservation of energy at discrete level. Let us consider the extended system in the x_1 direction

$$\rho\, c\, \frac{\partial T}{\partial t} = \frac{\partial \bar h}{\partial x_1}, \quad h = æ_{11}\, \frac{\partial \bar T}{\partial x_1} + g,$$

where the unknown functions are $\bar T \neq T$ and $\bar h \neq h$. For this system, the energy balance equation

$$\frac{\rho\, c}{2}\,\frac{\partial T^2}{\partial t} + æ_{11}\left(\frac{\partial \bar T}{\partial x_1}\right)^2 = \frac{\partial \bar h}{\partial x_1}\,(T-\bar T) + \frac{\partial \bar T}{\partial x_1}\,(h-\bar h) + \frac{\partial(\bar T\bar h)}{\partial x_1} - g\,\frac{\partial \bar T}{\partial x_1}. \tag{11}$$

is satisfied. It is transformed into a dissipative inequality

$$\frac{\rho\, c}{2}\,\frac{\partial T^2}{\partial t} + æ_{11}\left(\frac{\partial \bar T}{\partial x_1}\right)^2 \leqslant \frac{\partial(\bar T\bar h)}{\partial x_1} - g\,\frac{\partial \bar T}{\partial x_1}.$$

The closing equations of the extended system take the form

$$\begin{bmatrix} T-\bar T \\ h-\bar h \end{bmatrix} = -\,D \begin{bmatrix} \dfrac{\partial \bar h}{\partial x_1} \\ \dfrac{\partial \bar T}{\partial x_1} \end{bmatrix}, \quad D = \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix},$$

where D is a positive definite matrix. The discrete analogue of the extended system is the "corrector" step of the finite difference scheme:

$$\rho\, c\, \frac{T^{i_1} - T_{i_1}}{\Delta t/2} = \frac{h_{i_1+\frac12} - h_{i_1-\frac12}}{\Delta x_1}, \quad h_{i_1} = æ_{11,i_1}\, \frac{T_{i_1+\frac12} - T_{i_1-\frac12}}{\Delta x_1} + g_{i_1}. \tag{12}$$

For a more brief notation, there are no indices of the second direction, the upper indices correspond to the current time step, the lower indices correspond to the previous one, Δx_1, h_i and $æ_{11}$ are the spatial step, fluxes with mixed derivatives and the thermal conductivity coefficient in the x_1 direction. The quantities g_i are calculated explicitly using the values from the previous time step, and they include mixed derivatives with the coefficient æ$_{12}$. The solution is constructed with the time step $\Delta t/2$ as required for the splitting stages. The discrete analogue of equation (11) is

$$\rho\, c\, \frac{(T^{i_1})^2 - (T_{i_1})^2}{\Delta t} + æ_{11,i}\left(\frac{T_{i_1+\frac{1}{2}} - T_{i_1-\frac{1}{2}}}{\Delta x_1}\right)^2 = \frac{h_{i_1+\frac{1}{2}} - h_{i_1-\frac{1}{2}}}{\Delta x_1}\left(\frac{T^{i_1} + T_{i_1}}{2} - \frac{T_{i_1+\frac{1}{2}} + T_{i_1-\frac{1}{2}}}{2}\right) +$$
$$+ \frac{T_{i_1+\frac{1}{2}} - T_{i_1-\frac{1}{2}}}{\Delta x_1}\left(h_{i_1} - \frac{h_{i_1+\frac{1}{2}} + h_{i_1-\frac{1}{2}}}{2}\right) + \frac{(Th)_{i_1+\frac{1}{2}} - (Th)_{i_1-\frac{1}{2}}}{\Delta x_1} - g_{i_1}\frac{T_{i_1+\frac{1}{2}} - T_{i_1-\frac{1}{2}}}{\Delta x_1}.$$

The closing equations take the form

$$\begin{bmatrix} T^{i_1} + T_{i_1} - T_{i_1+\frac{1}{2}} - T_{i_1-\frac{1}{2}} \\ 2\, h_{i_1} - h_{i_1+\frac{1}{2}} - h_{i_1-\frac{1}{2}} \end{bmatrix} = \frac{-2\, D}{\Delta x_1}\begin{bmatrix} h_{i_1+\frac{1}{2}} - h_{i_1-\frac{1}{2}} \\ T_{i_1+\frac{1}{2}} - T_{i_1-\frac{1}{2}} \end{bmatrix}.$$

For simplicity, matrix D with one non-zero element with free parameter d is used: $D_{11} = = d - \Delta t / c\, \Delta x_1 \geqslant 0$ since the scheme approximates the heat conduction equation only with small elements of this matrix. The closing equations take the form

$$T_i - \frac{T_{i_1+\frac{1}{2}} + T_{i_1-\frac{1}{2}}}{2} = -\, d\, \frac{h_{i_1+\frac{1}{2}} - h_{i_1-\frac{1}{2}}}{2}, \quad g_{i_1} + æ_{11,i_1}\frac{T_{i_1+\frac{1}{2}} - T_{i_1-\frac{1}{2}}}{\Delta x_1} = \frac{h_{i_1+\frac{1}{2}} + h_{i_1-\frac{1}{2}}}{2}.$$

The equations for heat fluxes are obtained by adding and subtracting the closing equations:

$$d\, h_{i_1 \pm \frac{1}{2}} = d\, æ_{11,i_1}\frac{T_{i_1+\frac{1}{2}} - T_{i_1-\frac{1}{2}}}{\Delta x_1} \pm \frac{T_{i_1+\frac{1}{2}} + T_{i_1-\frac{1}{2}}}{2} \pm T_{i_1} + d\, g_{i_1}.$$

The step "predictor" for temperature is calculated using three-point sweep method in each direction:

$$-\left(\frac{d\, æ_{11,i_1}}{\Delta x_1} - \frac{1}{2}\right) T_{i_1+\frac{1}{2}} + \left(1 + \frac{d\big(æ_{11,i_1} + æ_{11,i_1-1}\big)}{\Delta x_1}\right) T_{i_1-\frac{1}{2}} - \left(\frac{d\, æ_{11,i_1-1}}{\Delta x_1} - \frac{1}{2}\right) T_{i_1-\frac{3}{2}} =$$
$$= T_{i_1} + T_{i_1-1} + d\big(g_{i_1} - g_{i_1-1}\big).$$

The final step of the splitting stage is the "corrector" step of the Godunov scheme. Taking into account that temperature in the right part is already found, the unknown quantities are determined as follows

$$\rho\frac{\bar{v_1} - v_1}{\Delta t} = \frac{p_{i_1} - p_{i_1-1}}{2\Delta x_1}, \quad \rho\frac{\bar{v_2} - v_2}{\Delta t} = \frac{q_{i_1} - q_{i_1-1}}{2\Delta x_1}, \quad \frac{\bar{p} - p}{\Delta t} = -\kappa\frac{v_{1_{i_1}} - v_{1_{i_1-1}}}{2\Delta x_1} + \beta\frac{\bar{T} - T}{\Delta t},$$

$$\frac{\bar{q} - q}{\Delta t} = \alpha\frac{v_{2_{i_1}} - v_{2_{i_1-1}}}{2\Delta x_1}, \quad J\frac{\bar{\omega} - \omega}{\Delta t} = \frac{\mu_{1_{i_1}} - \mu_{1_{i_1-1}}}{2\Delta x_1}, \quad \frac{\bar{\mu_1} - \mu_1}{\Delta t} = \gamma\frac{\omega_{i_1} - \omega_{i_1-1}}{2\Delta x_1}.$$

The values with a bar denote the values at the current time step, without a bar - at the previous time step. The indices for the second direction $i_2 - 1/2$ are omitted for brevity. In the finite differences in time, the indices $i_1 - 1/2$, $i_2 - 1/2$ are also omitted. At the 2nd and 4th stages, system of acoustic equations (13) and heat conduction equation (14) for the direction x_2 are solved in a similar way:

$$\left\{\begin{aligned} \rho\,\frac{\partial v_1}{\partial t} &= -\,\frac{\partial q}{\partial x_2} \\ \frac{\partial q}{\partial t} &= -\,\alpha\,\frac{\partial v_1}{\partial x_2} \end{aligned}\right., \quad \left\{\begin{aligned} \rho\,\frac{\partial v_2}{\partial t} &= -\,\frac{\partial p}{\partial x_2} \\ \frac{\partial p}{\partial t} &= -\,\kappa\,\frac{\partial v_2}{\partial x_2} \end{aligned}\right., \quad \left\{\begin{aligned} J\,\frac{\partial \omega}{\partial t} &= \frac{\partial \mu_2}{\partial x_2} \\ \frac{\partial \mu_2}{\partial t} &= \gamma\,\frac{\partial \omega}{\partial x_2} \end{aligned}\right.. \tag{13}$$

$$\rho\,c\,\frac{\partial T}{\partial t} = \frac{\partial h_2}{\partial x_2} - \beta\,T\,\frac{\partial v_2}{\partial x_2}, \quad h_2 = æ_{12}\,\frac{\partial T}{\partial x_1} + æ_{22}\,\frac{\partial T}{\partial x_2}. \tag{14}$$

At the 3rd stage the equations

$$J\,\frac{\partial \omega}{\partial t} = 2\,q, \quad \frac{\partial \theta}{\partial t} = \omega, \quad \frac{\partial q}{\partial t} = -\,2\,\alpha\Big(\omega + \frac{q}{\eta}\Big), \quad \rho\,c\,\frac{\partial T}{\partial t} = \frac{2\,q^2}{\eta}.$$

are solved in accordance with the Crank–Nicholson scheme:

$$J\,\frac{\bar\omega - \omega}{\Delta t} = 2\,\frac{\bar q + q}{2}, \quad \frac{\bar\theta - \theta}{\Delta t} = \frac{\bar\omega + \omega}{2}, \quad \frac{\bar q - q}{\Delta t} = -\,2\,\alpha\bigg(\frac{\bar\omega + \omega}{2} + \frac{\bar q + q}{2\,\eta}\bigg), \quad \rho\,c\,\frac{\bar T - T}{\Delta t} = \frac{(\bar q + q)^2}{2\,\eta}.$$

The indices $i_1 - 1/2$, $i_2 - 1/2$ for the values at the previous time step q, ω, θ and T as well as at the current time step $\bar q$, $\bar\omega$, $\bar\theta$ and $\bar T$ are omitted for brevity. Calculations are performed using the following formulas

$$\bar q = \frac{J\,\eta - \Delta t\,\alpha\,(\Delta t\,\eta + J)}{J\,\eta + \Delta t\,\alpha\,(\Delta t\,\eta + J)}\,q - \frac{2\,\Delta t\,\alpha\,J\,\eta}{J\,\eta + \Delta t\,\alpha\,(\Delta t\,\eta + J)}\,\omega,$$

$$\bar\omega = \omega + \frac{\Delta t}{J}(\bar q + q), \quad \bar\theta = \theta + \frac{\Delta t}{2}(\bar\omega + \omega), \quad \bar T = T + \frac{\Delta t}{2\,\rho\,c\,\eta}(\bar q + q)^2.$$

3. Results of computations

The described algorithm was implemented using the CUDA parallel programming technology [11]. Numerical calculations were performed for the 5CB liquid crystal. Parameters of the liquid crystal are [12, 13] $\rho = 1022$ kg/m^3, $j = 0.03 \cdot 10^{-12}$ kg/m, $\kappa = 11.1$ GPa, $\alpha = 360$ Pa, $\beta = 0.3 \cdot 10^{-6}$ K^{-1}, $\gamma = 6 \cdot 10^{-12}$ N, $\eta = 0.036$ Pa · c, $c = 100$ J/(kg · K), $æ_{\|} = 0.226$ W/(m · K), $æ_{\perp} = 0.135$ W/(m · K).

A rectangular LC layer with dimensions of 200×80 μm was considered. The finite difference grid contains 640×256 cells. At the initial moment of time $T_0 = 297$ K and $\theta = \pi/2$. At the upper border the temperature is set as follows $T = T_0 + T' e^{-4(x_{i_1} - x_c)^2/x_r^2}$, where T' is some constant, x_c is the centre of load application, x_r is the radius of the load.

Fig. 1 shows the results of the action of four heat sources with the radius of 20 μm on the lower boundary. In this case, $x_c = (i - 0.5)lx_1/n$, where $n = 4$ is the number of heat sources, $i = 1, 2, 3, 4$. Fig. 2 demonstrates the propagation and reflection of pressure waves initiated in the heating region. Fig. 3 shows the vector field of velocities. Fig. 4 shows the results of the action of one heat source in the middle of the right boundary. The other parameters are similar to the previous case. Fig. 5 and Fig. 6 show the propagation of pressure waves and the vector field of velocities, respectively. In both cases, velocities change in accordance with the change in pressure. Tangential stress, angular velocity and moment stresses in this case are equal to zero. The rotation angle remains unchanged due to the absence of tangential stresses. Thus, within the framework of the described model it is impossible to change the orientation of nematic liquid crystal molecules by varying only temperature field.

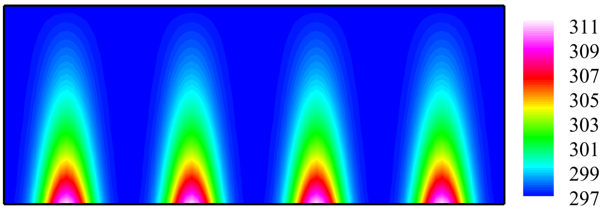

Fig. 1. Heating of the lower boundary: temperature level lines T, [K]

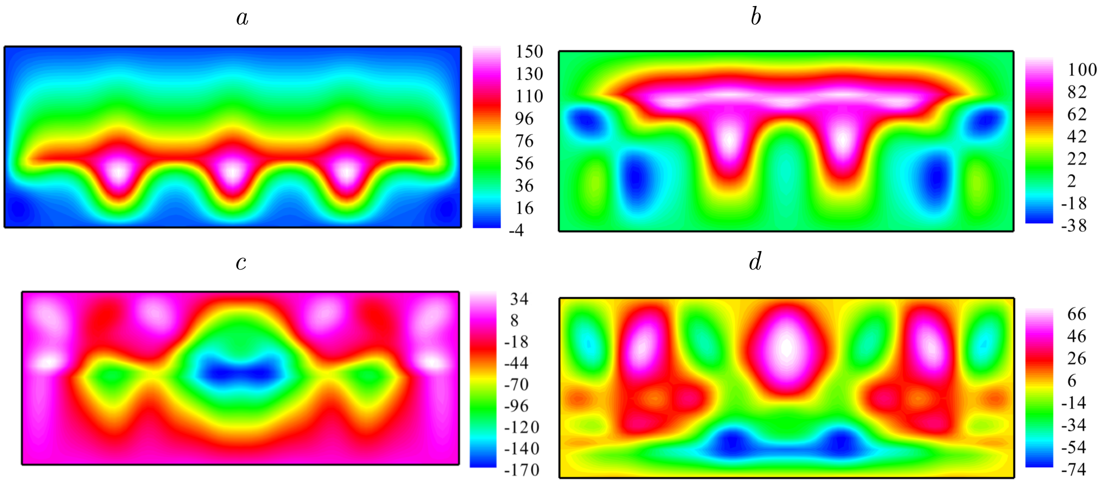

Fig. 2. Heating of part of the lower boundary: pressure level lines p, [nPa] (a — 9 ps, b — 18 ps, c — 36 ps, d — 45 ps)

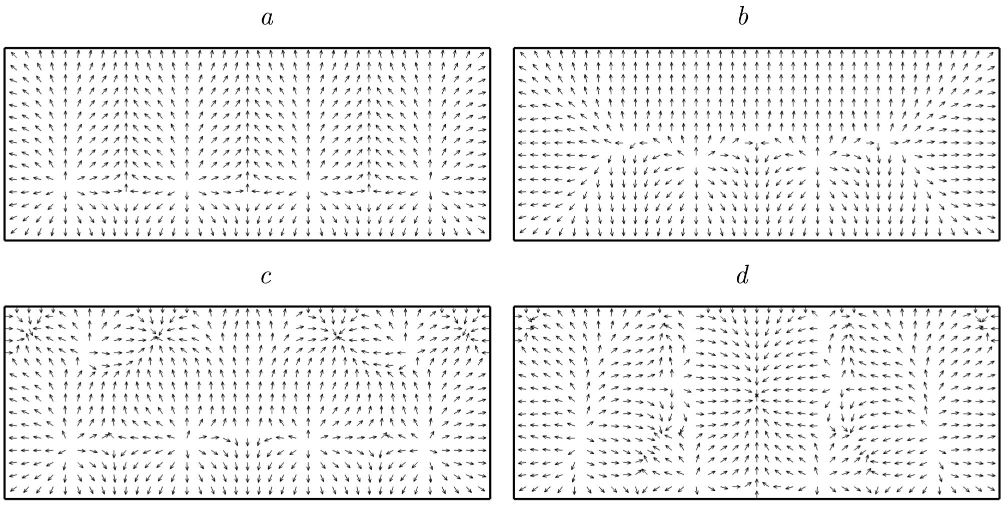

Fig. 3. Heating of part of the lower boundary: vector velocity field (a — 9 ps, b — 18 ps, c — 36 ps, d — 45 ps)

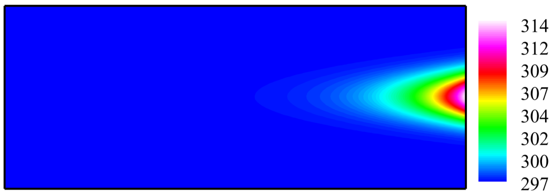

Fig. 4. Heating in the middle of the right boundary: temperature level lines T, [K]

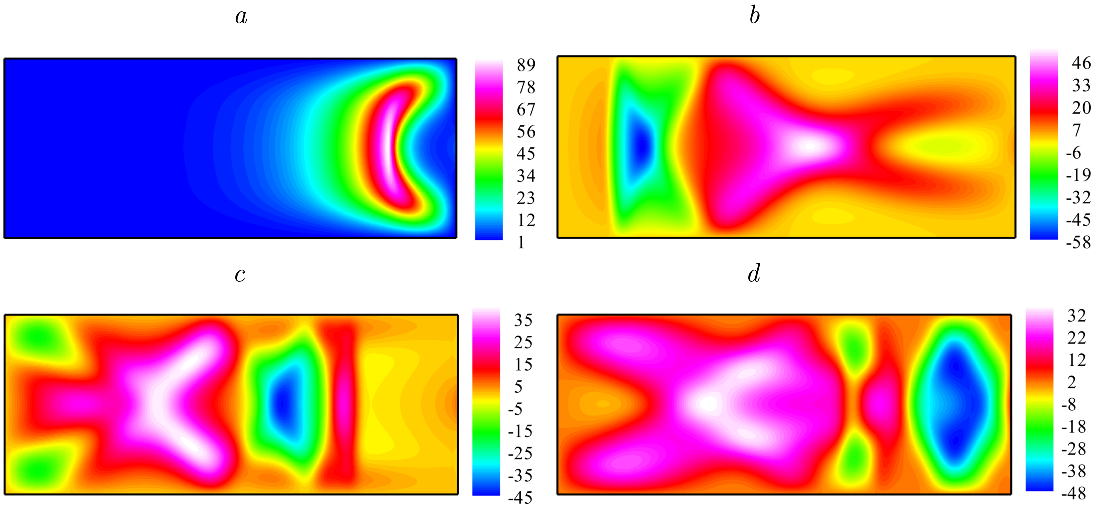

Fig. 5. Heating in the middle of the right boundary: pressure level lines p, [nPa] (a — 9 ps, b — 54 ps, c — 108 ps, d — 162 ps)

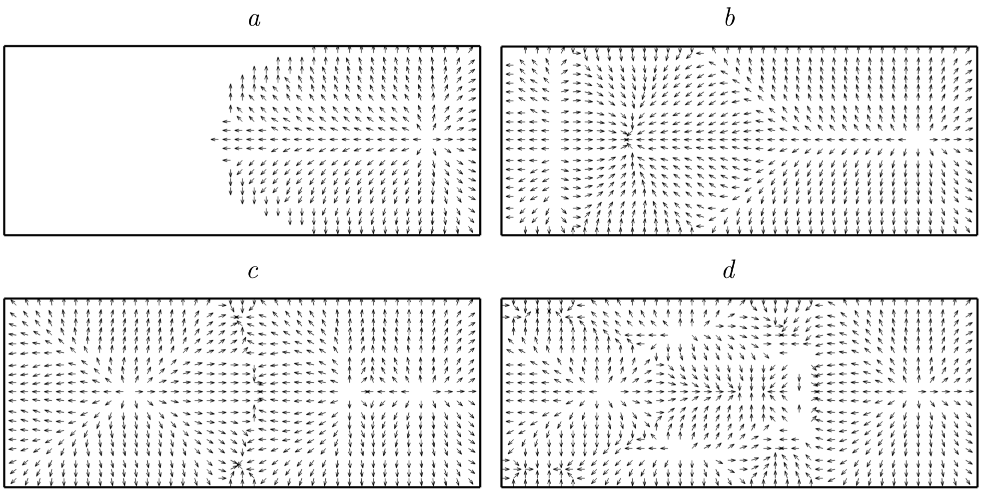

Fig. 6. Heating in the middle of the right boundary: vector velocity field (a — 9 ps, b — 54 ps, c — 108 ps, d — 162 ps)

Conclusion

The paper presents: a simplified model of thermomechanical and electrical effects in the acoustic approximation; an algorithm for numerical solution of the model equations; implementation of the algorithm as a parallel program in the C++ language with the help of the CUDA technology; a series of simulations that demonstrate that it is impossibile to observe the effect of orientational thermoelasticity using the presented dynamic model. It is assumed that if the surface tension forces will be taken into account then orientation of the molecules would change when one of the boundaries of the liquid crystal layer is heated.

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Исследование эффекта ориентационной термоупругости с помощью упрощенной модели нематического жидкого кристалла в акустическом приближении

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Аннотация. В работе представлен анализ эффекта ориентационной термоупругости с применением двумерной упрощенной динамической модели жидкого кристалла в акустическом приближении. Предполагается, что эффект возникает при нагревании одной из границ прямоугольного жидкокристаллического слоя. При решении системы уравнений модели применяется метод двуциклического расщепления по пространственным переменным в сочетании с конечно-разностной схемой распада разрыва Годунова для уравнений акустики и схемы Иванова с контролируемой диссипацией энергии для уравнения теплопроводности. Использование такой комбинации конечно-разностных схем позволяет проводить расчеты связанных термомеханических процессов с одинаковыми шагами по времени и по пространству, удовлетворяющими условию Куранта-Фридрихса-Леви. Численный алгоритм реализован в виде параллельной программы, написанной на языке C++. Распараллеливание вычислений выполнено для компьютеров с графическими ускорителями NVIDIA по технологии CUDA. Проведены расчеты, демонстрирующие невозможность наблюдения эффекта переориентации молекул жидкого кристалла под действием температуры для представленной упрощенной модели в акустическом приближении. Однако воздействие температуры существенно влияет на давление и скорости. Сделано заключение, что при учете сил поверхностного натяжения этот эффект будет наблюдаться для используемой в работе модели.

Ключевые слова: жидкий кристалл, теплопроводность, динамика, технология CUDA.