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Modeling of Electric Field Impact on a Cholesteric Liquid Crystal Layer

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Abstract. A new mathematical model is proposed to describe the spatial static state of a cholesteric liquid crystal. The model is constructed with the assumption of elastic resistance of a liquid crystal under weak mechanical action or under disturbance of electric field. Along with rotational degrees of freedom displacements of the centres of mass of the liquid crystal molecules relative to initial positions are taken into account. Using numerical calculations, the effect of deformation of cholesteric spirals in a thin layer under the action of electric field of a capacitor is analysed.

Keywords: cholesteric liquid crystal, statics, electric field, Fréedericksz effect.

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Introduction

It is common to divide natural and artificial liquid crystals into three classes. These classes include nematics, smectics and cholesterics. The centres of mass of molecules are randomly distributed in space in nematics but the direction vectors of molecules lie in the same plane. Smectics differ from nematics in a layered structure with abrupt/sharp boundaries of change in the orientation of molecules when moving from layer to layer. Cholesterics have a helical structure. The essential difference between these classes from the point of view of mathematical modelling is that under certain assumptions regarding external actions, two-dimensional models can be used to analyse nematics and smectics while two-dimensional models are not applicable to cholesterics. To simulate the deformation of liquid crystals in the cholesteric phase under the action of homogeneously distributed volumetric and surface forces and moments of forces it is necessary to use three-dimensional equations.

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Cholesterics are structurally similar to nematics. The molecules in cholesterics are arranged in thin layers in such a way that their long axes are parallel to each other, that is, a layer-by-layer orientation order is observed. But the presence of asymmetric (chiral) atoms in the molecules causes the molecules of the next layer to rotate through a small angle forming a helical structure (see Fig. 1). If we move along the helix axis then after a certain number of layers the orientation of the molecules becomes the same as in the first layer. One of the main characteristics of a cholesteric liquid crystal (ChLC) is the pitch of the cholesteric helix p_0 , i.e., the distance over which liquid crystal molecules rotate in space by the angle 2π . Another important characteristic of a liquid crystal is the director (vector) \vec{n} which determines the direction of the preferred orientation of the long axes of LC molecules.

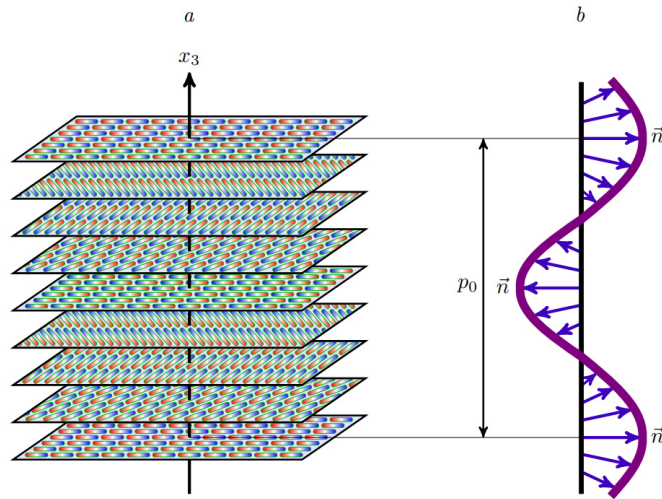


Fig. 1. Packing of rod-shaped molecules in cholesterics (a) and spiral arrangement of director \vec{n} (b)

The interaction of a cholesteric liquid crystal with bounding surfaces leads to the formation of various structures depending on the boundary conditions and the ratio of the helix pitch and the thickness of the drop or layer [1]. Various orientations of near-boundary molecules are provided at the stage of preliminary preparation of liquid crystal with the help of special technological processes. Orientation structures in cholesteric droplets and their optical textures were studied, for example, in [2,3]. Oriented ChLCs have a wide area of practical application as highly sensitive sensors based on colour changes, thermal indicators, reflectors, notch filters, polarizers and optical rotators, lasers, microlenses, etc. Detailed information about the current state of research on physical properties of cholesteric liquid crystals and technical devices based on them can be found in [4–6].

The theory of Eriksen–Leslie is used for mathematical modelling of liquid crystals (see, for example, [7]). It is applicable for solving static and non-stationary problems without restrictions on the flow structure. However, the complexity of non-linear equations of this theory is a significant obstacle to the development and justification of methods and algorithms for numerical implementation. Therefore, it is appropriate to apply approximate models that are based on simplifying hypotheses to solve specific problems.

We develop one of the approaches to model the behaviour of liquid crystals under the action of weak thermomechanical and electromagnetic perturbations. The model of acoustic approxi-

mation for the description of dynamic processes in liquid crystals was proposed [8]. Algorithms for numerical implementation of this model were developed and computations were performed for the layer of nematic liquid crystal (NLC) under the action of inhomogeneous electric field [9,10]. Computational algorithms for solving two-dimensional static problems were described [11]. The purpose of this paper is to create a simplified mathematical model of spatial deformation of a liquid crystal that is suitable for describing the cholesteric phase.

1. Mathematical model

The distribution of director in the liquid crystal relative to the Cartesian coordinate system x_1, x_2, x_3 with basis vectors $\vec{e}_1, \vec{e}_2, \vec{e}_3$ is given by a field of normals with orientation angles θ and ψ :

$$\vec{n} = \cos \theta \cos \psi \vec{e}_1 + \sin \theta \cos \psi \vec{e}_2 + \sin \psi \vec{e}_3 .$$

In the initial state of the ChLC layer $\psi = \psi_0$ and $\theta = \Delta\theta x_3/h$ that corresponds to helical structure with a given helix twist angle $\Delta\theta$ over the layer thickness h ($\psi_0 = 0$ in Fig. 2).

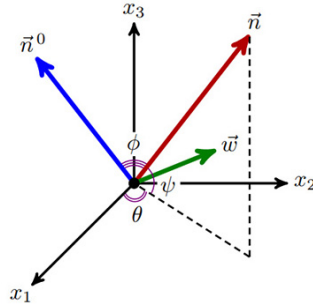


Fig. 2. Kinematic scheme of the rotational motion of director

Deformation caused by inhomogeneous external action at the boundary or inside the layer can lead to arbitrary change in both angles θ and ψ . Wherein a spatial stress-strain state is realized that is described on the basis of simplified equations of the Cosserat continuum under the assumption on hydrostatic state of a medium in the liquid phase. In this case, the stress tensor is represented by the components $\sigma_{jk} = -p\delta_{jk} + \tau_{jk}$, where p is the hydrostatic pressure, $\tau_{jk} = -\tau_{kj}$ are the components of antisymmetric tensor of tangential stresses, δ_{jk} is the Kronecker delta. Tangential stresses in a medium are due to the rotational degrees of freedom of the particles. In addition to tangential stresses the rotation of particles leads to the occurrence of couple stresses μ_{jk} which are the components of asymmetric tensor. Differential equations of equilibrium for an element of the medium take the following form

$$\frac{\partial p}{\partial x_k} - \frac{\partial \tau_{jk}}{\partial x_j} = f_k, \quad \frac{\partial \mu_{jk}}{\partial x_j} + \varepsilon_{ijk} \tau_{ij} = -m_k . \quad (1)$$

Here f_k и m_k are the projections of vectors of external body force and moment of force, ε_{ijk} is the Levi–Civita symbol. Einstein’s summation rule over repeated indices is accepted. Everywhere below the commonly accepted notations and operations of tensor analysis are used.

The governing equations of the model are obtained using the Castigliano variational principle. According to this principle the actual equilibrium state of the medium minimizes the

potential energy integral on the set of admissible states that satisfies equilibrium equations (1) and boundary conditions in stresses. These conditions are

$$-p \nu_k + \nu_j \tau_{jk} = \sigma_k^0 \quad \text{on} \quad S_\sigma, \quad \nu_j \mu_{jk} = \mu_k^0 \quad \text{on} \quad S_\mu, \quad (2)$$

where S_σ and S_μ are the parts of boundary S of domain V (layer, in a particular case), ν_k are projections of the outer normal vector to the boundary, σ_k^0 and μ_k^0 are the surface stresses given on S_σ and S_μ . The energy integral takes the form

$$J = \frac{1}{2} \int_V \left(\frac{1}{\kappa} p^2 + \frac{1}{\alpha} \tau_{jk} \tau_{jk} + \frac{1}{\gamma} \mu_{jk} \mu_{jk} \right) dV + \int_{S_u} u_k^0 (p \nu_k - \nu_j \tau_{jk}) dS - \int_{S_w} w_k^0 \nu_j \mu_{jk} dS.$$

Here κ , α and γ are phenomenological parameters of the medium: κ is the bulk compression modulus, α is the modulus of elastic resistance to relative rotation of particles, γ is the modulus of elastic resistance to curvature change; u_k^0 and w_k^0 are the displacements and rotations of particles that are set on the remaining parts of the boundary $S_u = S \setminus S_\sigma$ and $S_w = S \setminus S_\mu$, respectively.

The kinematic characteristics in the state of equilibrium (components of the displacement vector and the rotation vector in the case of the Cosserat continuum) are the Lagrange multipliers that corresponds to the constraints in the form of equilibrium equations. Therefore, the Lagrangian in the problem of conditional minimization under consideration can be represented as follows

$$L = J + \int_V \left(-u_k \frac{\partial p}{\partial x_k} + u_k \frac{\partial \tau_{jk}}{\partial x_j} + w_k \frac{\partial \mu_{jk}}{\partial x_j} + \varepsilon_{ijk} w_i \tau_{jk} \right) dV.$$

Equating to zero the variation of Lagrangian $\delta_p L = 0$, we obtain

$$\int_V \left(\frac{1}{\kappa} p \delta p - u_k \frac{\partial \delta p}{\partial x_k} \right) dV + \int_{S_u} u_k^0 \nu_k \delta p dS = 0.$$

After applying Green's formula, we have

$$\int_V \left(\frac{1}{\kappa} p + \frac{\partial u_k}{\partial x_k} \right) \delta p dV + \int_{S_u} (u_k^0 - u_k) \nu_k \delta p dS = 0.$$

Since variation δp is arbitrary we obtain equation and boundary condition

$$p = -\kappa \frac{\partial u_k}{\partial x_k}, \quad (u_k - u_k^0) \nu_k = 0 \quad \text{on} \quad S_u. \quad (3)$$

Similarly, the equality $\delta_{\tau_{jk}} L = 0$ implies that

$$\int_V \left(\frac{1}{\alpha} \tau_{jk} - \frac{\partial u_k}{\partial x_j} + \varepsilon_{ijk} w_i \right) \delta \tau_{jk} dV + \int_{S_u} (u_k - u_k^0) \nu_j \delta \tau_{jk} dS = 0.$$

Hence, taking into account boundary condition (3) and the antisymmetry of variation $\delta \tau_{jk} = -\delta \tau_{kj}$, the following equations and boundary condition are obtained

$$\tau_{jk} = \frac{\alpha}{2} \left(\frac{\partial u_k}{\partial x_j} - \frac{\partial u_j}{\partial x_k} - 2 \varepsilon_{ijk} w_i \right), \quad u_k = u_k^0 \quad \text{on} \quad S_u. \quad (4)$$

The equality $\delta_{\mu_{jk}} L = 0$ leads to equations and boundary condition

$$\mu_{jk} = \gamma \frac{\partial w_k}{\partial x_j}, \quad w_k = w_k^0 \quad \text{on} \quad S_w. \quad (5)$$

With an appropriate choice of phenomenological parameters of the medium system of equations and boundary conditions (1)–(5) is a closed mathematical model of the spatial deformation of the liquid crystal. To reduce it to a compact vector form the antisymmetric tangential stress tensor

$$\begin{pmatrix} 0 & -\tau_{21} & \tau_{13} \\ \tau_{21} & 0 & -\tau_{32} \\ -\tau_{13} & \tau_{23} & 0 \end{pmatrix},$$

is identified with the pseudovector

$$\vec{\tau}^\times = \tau_{32} \vec{e}_1 + \tau_{13} \vec{e}_2 + \tau_{21} \vec{e}_3 = -\varepsilon_{ijk} \tau_{jk} \vec{e}_i.$$

Then $\tau_{jk} = -\varepsilon_{ijk} \tau_i^\times$, $\nu_j \tau_{jk} \vec{e}_k = -\varepsilon_{ijk} \nu_j \tau_i^\times \vec{e}_k = \varepsilon_{ijk} \nu_j \tau_k^\times \vec{e}_i = \vec{\nu} \times \vec{\tau}^\times$,

$$\frac{\partial \tau_{jk}}{\partial x_j} \vec{e}_k = -\varepsilon_{ijk} \frac{\partial \tau_i^\times}{\partial x_j} \vec{e}_k = \varepsilon_{ijk} \frac{\partial \tau_k^\times}{\partial x_j} \vec{e}_i = \nabla \times \vec{\tau}^\times, \quad \nabla \times \vec{u} = \varepsilon_{ijk} \frac{\partial u_k}{\partial x_j} \vec{e}_i.$$

Using these relations, differential equations included in (1)–(5) are transformed to the following form

$$\begin{aligned} \nabla p - \nabla \times \vec{\tau}^\times &= \vec{f}, & p &= -\kappa \nabla \cdot \vec{u}, & \vec{\tau}^\times &= \alpha \left(\vec{w} - \frac{1}{2} \nabla \times \vec{u} \right), \\ -\nabla \cdot \vec{\mu} + 2 \vec{\tau}^\times &= \vec{m}, & \vec{\mu} &= \gamma \nabla \vec{w}. \end{aligned} \quad (6)$$

Boundary conditions for displacements and rotation angles obtained from the Castigliano variational principle have the following vector form

$$\vec{u} = \vec{u}^0 \quad \text{on } S_u, \quad \vec{w} = \vec{w}^0 \quad \text{on } S_w. \quad (7)$$

Boundary conditions (2) for stresses and couple stresses are as follows

$$-p \vec{\nu} + \vec{\nu} \times \vec{\tau}^\times = \vec{\sigma}^0 \quad \text{on } S_\sigma, \quad \vec{\nu} \cdot \vec{\mu} = \vec{\mu}^0 \quad \text{on } S_\mu. \quad (8)$$

Equations (6) with boundary conditions (7), (8) can be used to model the deformation of liquid crystal occupying an arbitrary domain under sufficiently general external actions of mechanical, temperature or electromagnetic fields inside the domain and on its boundary.

Let us consider the case of a non-magnetic liquid crystal (dielectric) when the bulk forces and moments of forces are caused by the action of an inhomogeneous electric field.

2. The action of electric field

The inhomogeneity of electric field is directly connected with the previously unknown orientation of LC molecules in a deformed state. Orientation, in its turn, depends on the electric field direction. The electric field \vec{E} is defined in terms of the spatial distribution of the electric potential φ : $\vec{E} = -\nabla \varphi$. In the absence of bulk electric charges inside domain V , the equation for the potential takes the form:

$$\nabla \cdot \vec{D} = 0, \quad \vec{D} = \boldsymbol{\varepsilon} \cdot \vec{E} \implies \nabla \cdot (\boldsymbol{\varepsilon} \cdot \nabla \varphi) = 0. \quad (9)$$

Here \vec{D} is the electric induction vector, $\boldsymbol{\varepsilon}$ is the dielectric permittivity tensor. It is defined as

$$\boldsymbol{\varepsilon} = \varepsilon^\perp \mathbf{I} + \Delta \varepsilon \vec{n} \vec{n},$$

where ε^{\parallel} and ε^{\perp} are permittivities along and across molecules, respectively, \mathbf{I} is the unit tensor, $\Delta\varepsilon = \varepsilon^{\parallel} - \varepsilon^{\perp}$.

The spatial distribution of the director \vec{n} depends on the electric field indirectly through the molecular rotation vector \vec{w} . When rotating through an infinitesimal angle, one can write

$$\vec{n} = \vec{n}^0 + \vec{w} \times \vec{n}^0. \quad (10)$$

This relation has a simple geometric interpretation (see Fig. 2). The projection $w_n = \vec{w} \cdot \vec{n}^0$ of the rotation vector onto the initial direction of the director describes the rotation of a medium around the \vec{n}^0 axis. Such rotation has no effect on the distribution of mechanical stresses and electric field since individual LC molecules are represented as rectilinear rigid needles of nanoscale length with negligible thickness. Vector $\vec{w} - w_n \vec{n}^0$ is orthogonal to the direction \vec{n}^0 and it describes the rotation of director from the initial position to the current one. Therefore, $\vec{w} - w_n \vec{n}^0 = \vec{n}^0 \times \vec{n}$. It is consistent with relation (10):

$$\vec{n}^0 \times \vec{n} = \vec{n}^0 \times \vec{n}^0 + \vec{n}^0 \times (\vec{w} \times \vec{n}^0) = \vec{w} (\vec{n}^0 \cdot \vec{n}^0) - \vec{n}^0 (\vec{n}^0 \cdot \vec{w}) = \vec{w} - w_n \vec{n}^0.$$

For finite rotations relation (10) is not applicable because condition $\vec{n}^2 = 1$ is violated. In this case, $\vec{n} = \mathbf{R} \cdot \vec{n}^0$, where \mathbf{R} is the rotation tensor that is defined in terms of the unit vector of the rotation axis

$$\vec{q} = \frac{\vec{w}}{|\vec{w}|} = \frac{\vec{n}^0 \times \vec{n}}{|\vec{n}^0 \times \vec{n}|}$$

and the rotation angle ϕ as follows

$$\mathbf{R} = \mathbf{I} + \sin \phi \mathbf{Q} + (1 - \cos \phi) \mathbf{Q}^2, \quad \mathbf{Q} = \begin{pmatrix} 0 & -q_3 & q_2 \\ q_3 & 0 & -q_1 \\ -q_2 & q_1 & 0 \end{pmatrix}.$$

If rotation occurs in the positive direction of vector \vec{w} then $\phi = |\vec{w}|$. If rotation takes place in the negative direction then $\phi = -|\vec{w}|$.

Contrary to traditional mathematical models of LC deformation in this model the director \vec{n} , which is required to calculate the dielectric permittivity tensor, does not belong to the main required functions. It is determined using rotation vector \vec{w} by relation (10) or by the more precise relation $\vec{n} = \mathbf{R} \cdot \vec{n}^0$.

Let us note that differential equation (9) is not sufficient to uniquely define the electric potential in V since the electric potential must be determined in the entire space including the exterior of V . If there are no bulk electric charges in the surrounding space and if it is filled with air or other rarefied gas with dielectric permittivity close to unity then the potential in it satisfies the Laplace equation $\nabla^2 \varphi = 0$. Moreover, it tends to zero at infinity. At the same time, conditions for continuity of the electric potential and the component of the electric induction vector normal to the interface are satisfied at the interface between the dielectric and the gas. It is also necessary to add to equation (9) boundary conditions on boundary S or on its part simulating the occurrence of non-zero electric field.

When potential is given the vector of bulk forces caused by the inhomogeneity of electric field is determined as follows

$$\vec{f} = (\vec{P} \cdot \nabla) \vec{E}, \quad \vec{P} = \varepsilon_0 \boldsymbol{\chi} \cdot \vec{E}, \quad \boldsymbol{\chi} = \boldsymbol{\varepsilon} - \mathbf{I},$$

where χ is the dielectric susceptibility tensor, \vec{P} is the polarization vector, $\varepsilon_0 = 8.854 \cdot 10^{-12}$ F/m is the electrical constant. In expanded form it becomes

$$\vec{f} = \varepsilon_0 \left((\varepsilon^\perp - 1) \nabla \varphi \cdot \nabla + \Delta \varepsilon (\vec{n} \cdot \nabla \varphi) \vec{n} \cdot \nabla \right) \nabla \varphi. \quad (11)$$

To determine the vector of moment of bulk forces the following relation is used

$$\vec{m} = \vec{P} \times \vec{E} \implies \vec{m} = \varepsilon_0 \Delta \varepsilon (\vec{n} \cdot \nabla \varphi) \vec{n} \times \nabla \varphi \quad (12)$$

It follows from (11) and (12) that LC molecules are subjected to bulk moments of forces in an arbitrary electric field, not excluding the case when field vector \vec{E} is constant everywhere in V , while bulk forces appear only with a non-uniform distribution of this vector.

3. One-dimensional problem

Let us consider LC layer of thickness h infinite in the plane x_1, x_2 between extended capacitor plates. Initial distribution of molecular orientation angles inside the layer is known: $\theta_0(x_3) = \Delta \theta x_3/h$, $\psi_0 = \psi_0(x_3)$. It corresponds to the cholesteric phase with the turn of spirals across the layer at an angle $\Delta \theta$. Molecules are reoriented when charges appear on the capacitor plates under the action of electric field.

Components of the dielectric permittivity tensor $\varepsilon_{jk} = \varepsilon^\perp \delta_{jk} + \Delta \varepsilon n_j n_k$ in the considered Cartesian coordinate system are

$$\begin{aligned} \varepsilon_{11} &= \varepsilon^\perp + \Delta \varepsilon \cos^2 \theta \cos^2 \psi, & \varepsilon_{12} &= \frac{1}{2} \Delta \varepsilon \sin 2\theta \cos^2 \psi, \\ \varepsilon_{22} &= \varepsilon^\perp + \Delta \varepsilon \sin^2 \theta \cos^2 \psi, & \varepsilon_{23} &= \frac{1}{2} \Delta \varepsilon \sin \theta \sin 2\psi, \\ \varepsilon_{33} &= \varepsilon^\parallel \sin^2 \psi + \varepsilon^\perp \cos^2 \psi, & \varepsilon_{13} &= \frac{1}{2} \Delta \varepsilon \cos \theta \sin 2\psi. \end{aligned}$$

In addition to reorientation, the layer is deformed under the action of electromagnetic forces. Taking into account the symmetry of the problem, we have

$$\vec{E} = -\varphi' \vec{e}_3, \quad \vec{P} = -\varepsilon_0 \varphi' \left(\varepsilon_{13} \vec{e}_1 + \varepsilon_{23} \vec{e}_2 + (\varepsilon_{33} - 1) \vec{e}_3 \right), \quad f_1 = f_2 = 0, \quad f_3 = \varepsilon_0 (\varepsilon_{33} - 1) \varphi' \varphi'',$$

and the prime denotes the derivative with respect to x_3 . The rotation of molecules is due to the action of moments of forces. Non-zero projections of the vector of moments are

$$m_1 = \frac{\varepsilon_0 \Delta \varepsilon}{2} (\varphi')^2 \sin \theta \sin 2\psi, \quad m_2 = -\frac{\varepsilon_0 \Delta \varepsilon}{2} (\varphi')^2 \cos \theta \sin 2\psi.$$

Vector \vec{m} at each point of the layer is turned out to be directed perpendicular to the plane passing through the director \vec{n} and the axis x_3 . This follows from the equality to zero of the scalar products $\vec{m} \cdot \vec{n} = \vec{m} \cdot \vec{e}_3 = 0$. Thus, the reorientation of molecules occurs only due to the change in angle ψ while angle $\theta = \theta_0(x_3)$ remains unchanged.

The differential equations of equilibrium for the layer take the form

$$-p' = f_3, \quad \mu'_{31} - 2\tau_1^\times = -m_1, \quad \mu'_{13} - 2\tau_2^\times = -m_2.$$

Non-zero projections of the rotation vector are

$$w_1 = \Delta \psi \sin \theta, \quad w_2 = -\Delta \psi \cos \theta \quad (\Delta \psi = \psi - \psi_0).$$

Constitutive equations for pressure, moment stresses and tangential stresses are

$$p = -\kappa u_3', \quad \mu_{31} = \gamma w_1', \quad \mu_{32} = \gamma w_2', \quad \tau_1^\times = \alpha w_1, \quad \tau_2^\times = \alpha w_2.$$

They allow one to transform the equilibrium equations to the following system of equations for displacement u_3 and rotation angle ψ

$$\kappa u_3'' = \varepsilon_0 (\varepsilon_{33} - 1) \varphi' \varphi'', \quad -2\gamma (\psi'' - \psi_0'') + 4\alpha (\psi - \psi_0) = \varepsilon_0 \Delta\varepsilon (\varphi')^2 \sin 2\psi. \quad (13)$$

Equation (9) for the electric potential is integrated as follows

$$(\varepsilon_{33} \varphi')' = 0 \quad \implies \quad \varphi' = \frac{C_1}{\varepsilon_{33}}.$$

The next condition is used to determine constant C_1

$$C_1 \int_0^h \frac{dx_3}{\varepsilon_{33}} = \Delta\varphi \quad (\varepsilon_{33} = \varepsilon^\parallel \sin^2 \psi + \varepsilon^\perp \cos^2 \psi), \quad (14)$$

where $\Delta\varphi$ is the difference of potentials on the capacitor plates.

After substituting expression for φ' and integrating the first equation (13), the system is transformed into

$$\kappa u_3' = -\varepsilon_0 C_1^2 \frac{1 - 2\varepsilon_{33}}{2\varepsilon_{33}^2} + C_2, \quad -2\gamma \Delta\psi'' + 4\alpha \Delta\psi = \varepsilon_0 C_1^2 \Delta\varepsilon \frac{\sin 2(\psi_0 + \Delta\psi)}{\varepsilon_{33}^2}. \quad (15)$$

The boundary conditions $\Delta\psi(0) = \Delta\psi(h) = 0$ are added to the equation for the angle of rotation. Such problem is solved numerically. The distribution $\psi^0(x_3) = \psi_0(x_3)$ is taken as the initial distribution of angles. According to the given distribution $\psi^n(x_3)$, the approximate value of constant C_1^n is calculated using (14). New approximation $\psi^{n+1}(x_3)$ is determined using three-point sweep method based on the iterative algorithm

$$-2\gamma \frac{\Delta\psi_{j+1}^{n+1} - 2\Delta\psi_j^{n+1} + \Delta\psi_{j-1}^{n+1}}{\Delta x_3^2} + 4\alpha \Delta\psi_j^{n+1} = \varepsilon_0 C_1^2 \Delta\varepsilon \frac{\sin 2(\psi_{0j} + \Delta\psi_j^n)}{(\varepsilon_{33j}^n)^2}. \quad (16)$$

The process is stopped when the condition $\|\Delta\psi^{n+1} - \Delta\psi^n\| / \|\Delta\psi^n\| < \delta$ is fulfilled, where $\|\Delta\psi\|$ is a uniform difference norm, δ is a given calculation error.

After finding constant C_1 using the trapezoid rule, potential φ is calculated from relation

$$\varphi(x_3) = C_1 \int_{h/2}^{x_3} \frac{dx_3}{\varepsilon_{33}}.$$

The equation for displacement is integrated numerically for boundary conditions of two types: $u_3(0) = u_3(h) = 0$ and $u_3(0) = 0, u_3'(h) = 0$. In the first case, constant C_2 is determined as

$$C_2 = \frac{\varepsilon_0 C_1^2}{2h} \int_0^h \frac{1 - 2\varepsilon_{33}}{\varepsilon_{33}^2} dx_3,$$

and in the second case as

$$C_2 = \varepsilon_0 C_1^2 \frac{1 - 2\varepsilon_{33}}{2\varepsilon_{33}^2} \Big|_{x_3=h}.$$

When initial angle $\psi_0 = 0$ is equal to zero equation (15) for the rotation angle describes the Fréedericksz effect of the loss of equilibrium of LC molecules in electric field. As a result of linearisation of the equation, the problem is reduced to the boundary value problem

$$\gamma h^2 \psi'' = (2\alpha h^2 \psi - \varepsilon_0 \Delta\varepsilon \Delta\varphi^2) \psi, \quad \psi(0) = \psi(h) = 0.$$

After substituting the solution $\psi = A \sin \pi x_3/h$, where A is an arbitrary constant, we obtain the formula for the difference of potentials at which the trivial solution becomes unstable

$$\Delta\varphi_0 = \sqrt{\frac{\pi^2 \gamma + 2 h^2 \alpha}{\varepsilon_0 \Delta\varepsilon}}. \quad (17)$$

In comparison with the classical formula for the Fréedericksz transition threshold, which takes into account only moment interactions, it contains a correction accounting the resistance to rotation of particles due to tangential stresses and it shows that such resistance prevents the loss of stability.

Formula (17) is used for verification of the algorithm and program. According to the results of computations of the liquid crystal with parameters $\varepsilon^{\parallel} = 16.7$, $\varepsilon^{\perp} = 7$, $\alpha = 2.45$ Pa, $\gamma = 6 \cdot 10^{-12}$ N and $\kappa = 3.12$ GPa the value of potential difference $\Delta\varphi = 1.27$ V is obtained which is close to the threshold value corresponding to the transition of the layer into unstable state. At smaller values of $\Delta\varphi$ the orientation of molecules calculated by scheme (16) with $\psi_0 = 0$ remains unchanged and $\psi = 0$. The electric potential is distributed linearly over the layer: $\varphi = (x_3/h - 0.5) \Delta\varphi$. For larger values of the difference of potentials the transition occurs from initial unstable state to a stable one which is characterized by inhomogeneous distribution of angle ψ and non-linear distribution of potential φ over the layer. There are two stable states that differ in the sign of the molecular orientation angle. The positive or negative sign is realized in computations. It depends on the small perturbation of the initial angle ψ_0 .

Let us note that the sequence of approximations of the orientation angle in the numerical implementation of scheme (16) is rapidly converges (number of iterations is about 10) if the resulting value of angle ψ at the layer centre is away from 90° , i.e., differs from the orientation angle of the electric field. When the value of angle ψ approaches 90° the convergence of the iterative process slows down with the transition to the divergent regime. In addition, the expansion of non-linear right-hand side (16) according to the Newton method does not allow one to expand the range of admissible setting of potential difference $\Delta\varphi$ in which the approximations converge but, on the contrary, leads to a significant narrowing this range.

4. Numerical results

The results of computations for the layer of thickness $h = 4 \mu\text{m}$ with potential difference $\Delta\varphi = 1.28$ V (it is close to the threshold value) are shown in Figs. 3–6. The curves of red, green, blue and violet colours in Fig. 3 demonstrate diagrams of the distribution of the orientation angle over the layer for initial values $\psi_0 \approx 0$, $\psi_0 = 5^\circ$, 10° and 15° . Deviations of potential from the linear distribution $\delta\varphi(x_3) = \varphi(x_3) - (x_3/h - 0.5) \Delta\varphi$ corresponding to these values are shown in Fig. 4. Results of computations demonstrate that potential distribution for small values of initial angle ψ_0 is close to linear distribution but it changes significantly with a slight change in this parameter.

Figs. 5 and 6 show diagrams of strain distribution $\varepsilon_{33} = u'_3$ for two types of boundary conditions on the sides of the layer (on capacitor plates). In both cases, the level of strains is

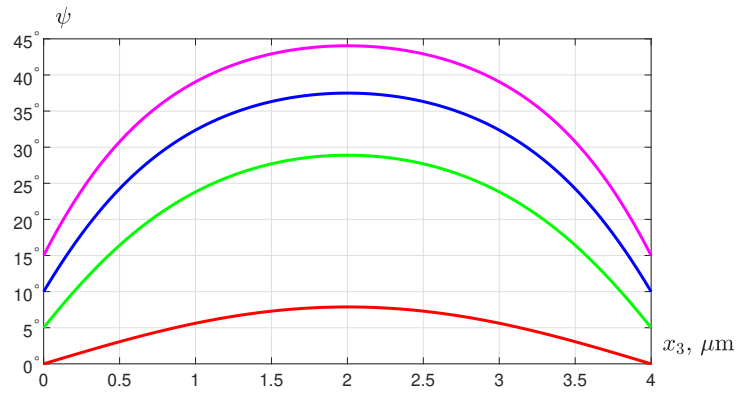


Fig. 3. Distribution of the rotation angles of molecules over the LC layer

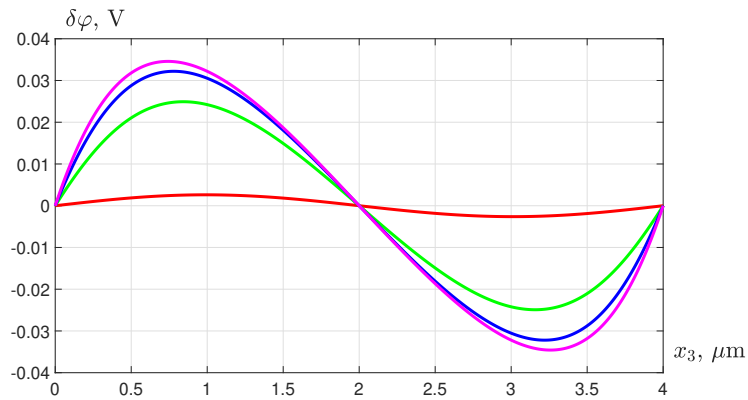


Fig. 4. Deviation of the electric potential from linear distribution

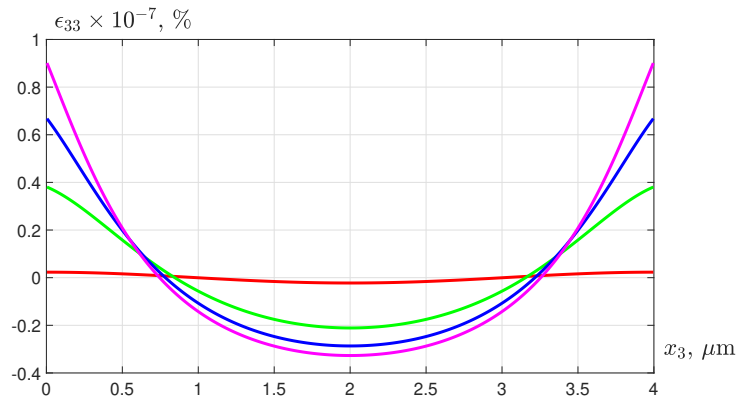


Fig. 5. Strain distribution over the LC layer for fixed sides

negligible (about 10^{-7} %) since the electric field in the problem under consideration is practically uniform. Its inhomogeneity is determined by a slight change in the LC dielectric permittivity due to relative rotation of molecules. Nevertheless, the following characteristic qualitative features

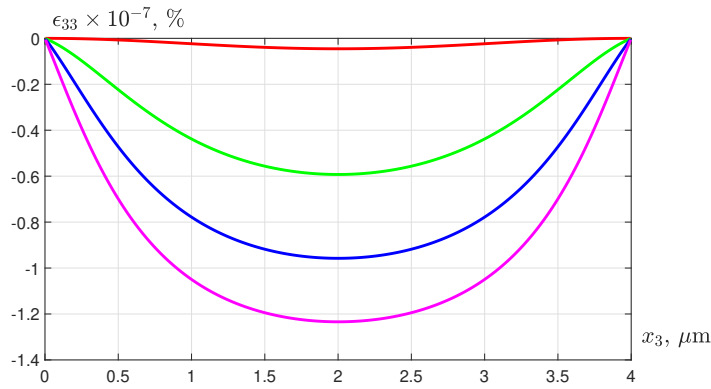


Fig. 6. Strain distribution over the LC layer for free surface

can be noted. If both sides are fixed, the layer is stretched near boundaries and compressed in the centre. Thus, the pitch of cholesteric helices of the liquid crystal is increased in comparison with the initial pitch near capacitor plates, and it is decreased in the middle part of the layer. Under the condition of a free surface, the layer is compressed everywhere but the pitch of helices is decreased in the centre, and it remains practically the same as in the initial undeformed state near the sides.

Results of computations presented in Fig. 7 correspond to the LC layer that consists of two sublayers of equal thickness. The initial orientation angles are $\psi_0 = 0$ (in the lower sublayer) and $\psi_1 = 5^\circ, 10^\circ, 15^\circ, 20^\circ$ (in the upper sublayer). Considering results of computations, one can see that jump in the orientation angle of molecules at the interface between sublayers after the application of constant electric field remains the same as it was set in the initial state. This follows directly from the analysis of equation (15) for the rotation angle. The right-hand side of the equation is discontinuous function with discontinuity of the first kind at the interface between sublayers.

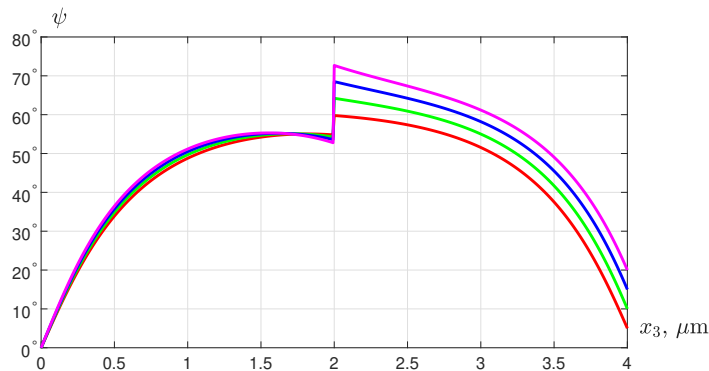


Fig. 7. Distribution of the rotation angles of molecules over the LC layer consisting of two sublayers

Performed computations demonstrate the applicability of the proposed mathematical model for calculating liquid crystals of a layered smectic phase.

Conclusion

To describe the static deformed state of the liquid crystal under the action of weak external perturbations a simplified mathematical model is proposed. The liquid crystal is considered as structurally inhomogeneous continuum with translational and rotational degrees of freedom of the micro-structure particles (LC molecules). This model is applicable to the analysis of cholesteric liquid crystals with spatial helical orientation of molecules. To demonstrate implementation of the model the problem of deformation of a cholesteric liquid crystal layer in the electric field of a capacitor was considered. The state of the liquid crystal in the vicinity of the Fréedericksz transition was studied numerically. Distributions of the orientation angle, electric potential and strain over the layer were obtained for various initial orientation angles. Analysis of the results of computations demonstrates that predominant compression of cholesteric spirals under the electric field action (its inhomogeneity over the layer is determined by the change in the dielectric permittivity due to the rotation of molecules) occurs in the middle part of the ChLC layer.

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Моделирование действия электрического поля на жидкокристаллический слой холестерика

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Аннотация. В рамках предположения об упругом сопротивлении холестерического жидкого кристалла слабым механическим воздействиям или возмущениям электрическим полем строится новая математическая модель для описания пространственного статического состояния. Наряду с вращательными степенями свободы учитываются смещения центров масс молекул жидкого кристалла относительно начального положения. С помощью численных расчетов в задаче для тонкого слоя анализируется эффект деформации холестерических спиралей под действием электрического поля конденсатора.

Ключевые слова: холестерический жидкий кристалл, статика, электрическое поле, эффект Фредерикса.