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Orientation Instability of the Layer of a Nematic Liquid Crystal

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Abstract—The origin of periodic structures in a layer of a lyotropic nematic liquid crystal observed in the director (vector, describing the anisotropic properties of the medium) reorientation experiment is studied. Such perturbations with the wavevector perpendicular to the initial orientation can develop in a liquid crystal layer in the unstable equilibrium state when the director is parallel to the walls under the condition that its orthogonality to the boundary corresponds to the minimum anchoring energy. It is shown that the linear dependence of the domain period on the layer thickness observed experimentally can be theoretically described when the Frank orientation elasticity energy is considered in the most general form taking the divergence terms into account and the anchoring energy of orientation is small as compared with the bulk energy. A relation between the coefficient of the divergence terms (saddle-splay elastic constant) and two other coefficients in the Frank energy is obtained.

Keywords: anchoring energy, nematic liquid crystals, orientation, instability.

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Media in which the molecules and other base units are strongly elongated can be related to the class of nematic liquid crystals. In this case, a mean direction of orientation of the major axes described by a unit vector $\mathbf{n}$ called the director [1] exists in the liquid-crystal phase. The presence of an additional macroscopic parameter leads to appearance of the internal energy of the Frank orientation elasticity which in the most generic case with allowance for the properties of symmetry of the medium including the equivalence of the directions $\mathbf{n}$ and $-\mathbf{n}$ takes the form:

$$2F_V = K_1(\operatorname{div}\mathbf{n})^2 + K_2(\mathbf{n},\, \operatorname{curl}\mathbf{n})^2 + K_3\big|[\mathbf{n},\, \operatorname{curl}\mathbf{n}]\big|^2$$

$$+ K_{24}\big(\nabla_i n_j \nabla^j n^i - (\nabla_k n^k)^2\big),$$

the constant coefficients K_i are the Frank constants. In this case the last term has the divergence form by virtue of the identity $\nabla_i n_j \nabla^j n^i - (\nabla_k n^k)^2 \equiv \nabla_i(n^j \nabla_j n^i - n^i \nabla_k n^k)$ and has no effect on the equations of motion or equilibrium of the medium and the equation of the director orientation. However, this term must be taken into account in the boundary conditions (weak anchoring) when the orientation vector is not given on the boundary but can be found from the condition of minimum anchoring energy. Usually, the anchoring energy is given by the Papini–Papoular relation [2]

$$F_S = \gamma + \frac{W}{2}\big(1 - (\sin\Omega\sqrt{1 - n_m^2} + \cos\Omega|n_m|)^2\big),$$

where $n_m = (\mathbf{n},\, \mathbf{m})$, $\mathbf{m}$ is the unit outward normal to the boundary, γ, W, and Ω are constants, and Ω is the angle between the light orientation axis and the normal to the surface ($\Omega \in [0,\, \pi/2]$).

In [3–5] it was shown that taking the divergence terms in the Frank energy into account can lead to instability of surface waves with the free boundary. In [6–11] the role of these terms was studied for a liquid crystal layer in the equilibrium state which is enclosed between two rigid walls. It was found that nontrivial periodic solutions can exist in the presence of such terms in the case of a layer with plane boundaries and homogeneous boundary conditions. The question of the effect of the layer thickness and the relation between the Franc coefficients on the existence of such solutions and their number was also considered in these studies. In [12] there was proposed a method of measuring the saddle-splay elastic constant K_{24} based on studying periodic structures arising in the nematic layer under the action of a magnetic field.

In [13] domain structures developed in the layer of a lyotropic nematic liquid crystal (disulfoindantron-water system) in the process of transition of the director from the planar (parallel to the walls) to homeotropic (perpendicular to the boundaries) orientation were described. In Fig. 1 we have reproduced the schematic diagram of the experiment. In the initial state (in filling the cell), the planar orientation develops in the layer due to the action of viscous forces (zone II in Fig. 1). In this case the homeotropic orientation corresponds to the minimum anchoring energy for the system under consideration. In a certain time homeotropic domains (zone I in Fig. 1) begin to develop in the stopped medium. In those cases, in which the boundaries of the reoriented domains were perpendicular to the initial director position, periodic domain structures develop in the undisturbed zone in a time of the order of several minutes. Their wavevector was perpendicular to the orientation vector. These structures were recorded experimentally in the form of dark stripes in the zone with planar orientation. In this study it was noted that for the layer in a cell the total reorientation time was equal to approximately one hour while the domain structure existence time amounts to from several to tens minutes. In this case the domain period did not vary during all time of propagation of the reorientation front and agreed within a good accuracy with the layer thickness varied from 30 to 200 μm. In [13] a dynamic description of the effects observed was proposed and the effect of various forces was estimated by means of the dimension theory. In the present study a possible theoretical description of the origin of such structures due to taking the divergence terms in the Frank energy into account is proposed.

1. FORMULATION OF THE PROBLEM ON EQUILIBRIUM OF THE LAYER

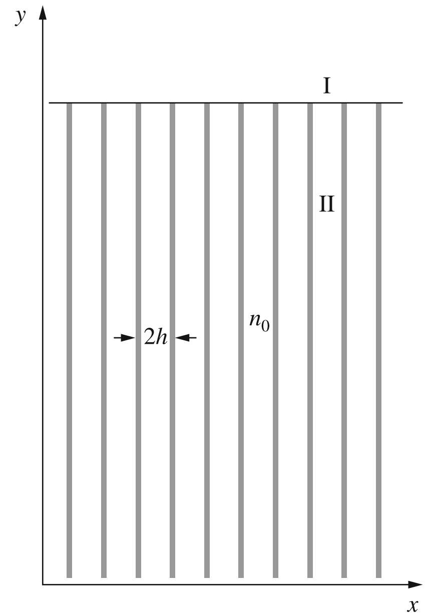
For the problem of nematic equilibrium the equations governing the director field in the absence of external body forces and the weak anchoring take the form [14]:

$$\left(\delta_k^j - n^j n_k\right)\left(\frac{\partial F_V}{\partial n^j} - \nabla_i\left(\frac{\partial F_V}{\partial \nabla_i n^j}\right)\right) = 0, \tag{1.1}$$

$$\left(\delta_k^j - n^j n_k\right)\left(\frac{\partial F_V}{\partial \nabla_i n^j} m_i + \frac{dF_S}{dn_m} m_j\right) = 0. \tag{1.2}$$

In this case the pressure can be found from the equation $\nabla_i(p + F_V) = 0$ after the director field has been determined and the boundary conditions have been specified. Equations (1.1) and (1.2) are projected on the plane orthogonal to the vector $\mathbf{n}$ to eliminate the indefinite Lagrange multipliers that appear owing to the condition of its constant length.

We will consider the plane problem of equilibrium of the layer of a nematic liquid crystal that occupies the gap between the planes $z = \pm h$ in the Cartesian coordinate system $(x,\ y,\ z)$ with the undisturbed homogeneous director orientation $\mathbf{n} = (0,\ 1,\ 0)$. In the disturbed state the director is given as follows: $\mathbf{n} = (-\sin\varphi\cos\theta,\ \cos\varphi\cos\theta,\ -\sin\theta)$, where φ and θ are the angles of deviation from the initial direction of the director. Then the linearized equilibrium equations (1.1) for perturbations of the angles φ and θ,



Pattern of the domain under consideration: zone I corresponds to orientation of the director perpendicularly to the *Oxy* plane and zone II to the initial planar domain; $2h$ is the domain period.

which were obtained analogously in [6] for another initial state of the director, can be written as follows:

$$K_2\theta_{xx} + K_1\theta_{zz} = (K_2 - K_1)\varphi_{xz}, \tag{1.3}$$

$$K_1\varphi_{xx} + K_2\varphi_{zz} = (K_2 - K_1)\theta_{xz}. \tag{1.4}$$

In this case, owing to the properties of the investigated medium, which were established in [15, 16], in Eqs. (1.3), (1.4) we will consider the most general case for the Frank energy in which the constants K_i are different and the quantity K_3 does not enter into the equations.

The weak anchoring can be reduced to the relations

$$K_2\,\varphi_z = \theta_x\big(K_2 - K_{24}\big), \tag{1.5}$$

$$K_1\,\theta_z - \varphi_x\big(K_{24} - K_1\big) = \pm W\theta, \tag{1.6}$$

where the subscripts "x" and "z" denote the partial derivatives with respect to the corresponding coordinates. Condition (1.5) can be applied to both boundaries. In condition (1.6) the upper and lower signs relate to upper and lower boundaries, respectively. Since the undisturbed state corresponds to the maximum anchoring energy, equation (1.6) differs from the corresponding boundary conditions (weak anchoring) [10, 11] by opposite sign on the right-hand side.

2. NONTRIVIAL PERIODIC SOLUTIONS

We will seek the solutions for the undisturbed state in the form:

$$\theta = f(z)\sin kx, \qquad \varphi = g(z)\cos kx.$$

Then the system (1.3), (1.4) can be reduced to a fourth-order equations with constant coefficients, for example, for the functions $f(z)$. Its characteristic polynomial has the roots $\pm k$ of double multiplicity. The solutions for $f(z)$ and $g(z)$ can be written in the form:

$$g(z) = (A_1 + A_2 z)\exp(kz) + (A_3 + A_4 z)\exp(-kz),$$

$$f(z) = (D_1 + D_2 z)\exp(kz) + (D_3 + D_4 z)\exp(-kz),$$

where, by virtue of Eqs. (1.3), (1.4), the coefficients A_i and D_i are connected by the relations

$$A_2 = D_2, \qquad kA_1 - kD_1 = \lambda A_2, \tag{2.1}$$

$$A_4 + D_4 = 0, \qquad kA_3 + kD_3 = \lambda D_4, \tag{2.2}$$

$$\lambda = \frac{K_1 + K_2}{K_1 - K_2}.$$

The boundary conditions (weak anchoring) (1.5), (1.6) together with relations (2.1), (2.2) make it possible to write a linear homogeneous system for the coefficients A_i and D_i. The condition of existence of a nontrivial solution of this system (its determinant must be equal to zero) leads to the equation

$$\begin{gathered} -4k^6K_{24}^4h^2 + k^4\big\{-4hK_2W(\lambda + 1) + \sinh^2(2kh)\zeta\big\}K_{24}^2 \\ + k^3K_{24}K_2W\xi\sinh(4kh) + k^2W^2K_2^2\sinh^2(2kh)(\lambda + 1)^2 = 0, \\ \zeta = (\lambda K_{24} - \lambda K_1 - \lambda K_2 + K_1 - K_2)^2, \\ \xi = \lambda(\lambda + 1)K_{24} - K_2 + K_1 - 2\lambda K_2 - \lambda^2K_2 - \lambda^2K_1. \end{gathered} \tag{2.3}$$

From relation (2.3) it follows that the presence of the divergence terms in the Frank energy is necessary for existence of nontrivial solutions which are absent when $K_{24} = 0$. We will use the experimental data [13]; hence, with allowance for the form of the solution and the property of equivalence of the directions $\mathbf{n}$ and $-\mathbf{n}$ we can set $2kh = \pi$. In that study it was also noted that the surface forces affect the medium only slightly. This is confirmed by the fact that the director in a cell changes its orientation over a long period of time. For example, this can be related to the nature of interaction between the nematic and the boundary. In review [17] it was noted that in certain cases other approximations in which the anchoring energy for the director positions far from the axis of light orientation varies only slightly must be considered instead of the Papini–Papoular model. For example, the elliptic sine can be taken [18] as the function that describes the anchoring energy. In this case, if we set $W = 0$ in Eq. (2.3), this admits a linear relation between the perturbation wavelength and the layer thickness. Taking the experimental data into account, from this relation it follows that K_{24} is connected with other coefficients in the Frank energy as follows:

$$\pi^2K_{24}^2 = \sinh^2(\pi)(\lambda K_{24} - \lambda K_1 - \lambda K_2 + K_1 - K_2)^2.$$

The last relation can be used to determine the parameter K_{24}.

Summary. An approach which makes it possible to obtain solutions that describe periodic structures observed in the layer of a lyotropic nematic liquid crystal is proposed. It is shown that their existence is possible if the divergence terms are taken into account in the Frank orientation elasticity energy. A relation between the wavenumber, the layer thickness, and the Frank coefficients is obtained for the periodic solutions when the orientation energy is considered in the most general form admitted by the properties of symmetry of the medium, i.e., with four different constants. An investigation of this equation shows that the linear dependence of the perturbation period on the layer thickness is possible if the effect of the anchoring orientation energy on the medium boundary is negligibly small as compared with its bulk value. Taking the available experimental data into account, an equation relating the divergence constant in the Frank energy with three other constants is obtained.

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