About orientational instability in nematic liquid crystal films

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Abstract. In the presented work the role of the surfacelike (splay-bend) elastic constant in the Frank’s energy of nematic liquid crystals for orientational instability in the thin nematic films is considered. It is shown that nontrivial periodical perturbations exist in the nematic film with undisturbed planar director orientation in case of sufficiently large value of splay-bend constant. For these solutions the relations between splay-bend constant, another Frank’s constants and layer thickness are received and studied. These correlations allow us to make new explanation for certain experimental effects and to present method for surfacelike constant value measurement.

1. Introduction
The anisotropic properties of nematic liquid crystals (NLC) are described by unit vector \( \vec{n} \) (director). In case of Frank-Oseen-Leslie model the Frank’s volume free energy has the form

\[
2F_V = K_{11} (\text{div} \vec{n})^2 + K_{22} (\vec{n} \cdot \text{rot} \vec{n})^2 + K_{33} |[\vec{n} \times \text{rot} \vec{n}]|^2 + K_{24} \left( \nabla_i n_j \nabla_j n_i - (\nabla_k n^k)^2 \right)
\]  

where \( K_{ii} \) are the Frank’s constants [1]. On account of nematic symmetry only four independent constants exist, but discussion about Frank’s energy expression has a long history [2,3]. The last term in (1) has the divergent form and does not bring the contribution in the equations of continuum motion and director evolution or equilibrium, but it is necessary to take it into account together with the surface energy [4] in the boundary conditions in case of director weak anchoring on the nematic-isotropic interface. The Frank’s energy is the positive definite function if \( K_{ii} \) satisfy the Ericksen inequalities \( 2K_1 \geq K_{24} \geq 0, 2K_2 \geq K_{24} \geq 0, K_3 \geq 0 \) [1], but some nematics does not satisfy these conditions [5].

Scientific interest to the role of surfacelike part of Frank’s energy arose after Oldano-Barbero paradox (continuous solution for director field in the nematic layer does not exist for some boundary conditions) was discovered [6,7]. Instability induced by surfacelike constant \( K_{24} \) in the cylindrical pore is studied in [8,9], in the surface waves – in [10], works [11,12] deal with the periodical solutions in the hybrid aligned nematic sell. In the presented work we discuss the periodical solutions as perturbation of the homogeneous director field in the NLC film.
2. Formulation of the problem on equilibrium of NLC film

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 [13]

\[
\left( \delta_q^i - n^i n_q \right) \left( \frac{\partial F}{\partial n^q} - \nabla_k \left( \frac{\partial F}{\partial \nabla_k n^q} \right) \right) = 0
\] (2)

\[
\left( \delta_k^i - n^i n_k \right) \left( \frac{\partial F}{\partial n^q} m_i + \frac{dF_s}{dn_m} m_j \right) = 0
\] (3)

For surface energy Rapini–Papoular model is used [4]

\[
F_S = \gamma + \frac{W}{2} (1 - (\vec{n} \cdot \vec{m})^2) = \gamma + \frac{W}{2} (1 - (\sin \Omega \sqrt{1 - n^2} + \cos \Omega |n_\nu|)^2)
\] (4)

where \( n_m = \vec{n} \cdot \vec{m} \), \( \vec{m} \) is the unit outward normal to the boundary, \( \gamma \), \( W \), and \( \Omega \) are constants, and \( \Omega \) is the angle between the light orientation axis and the normal to the surface. In case of planar orientation for director on the boundary \( \Omega = \pi/2 \).

We consider the NLC film with undisturbed homogeneous director field \( \vec{n} = (0, 1, 0) \), because this configuration is the most unstable for perturbation in the \( xz \) plane [14]. In Cartesian coordinates this film is bounded by planes \( z = \pm h \). In the disturbed state the director is given as follows: \( \vec{n} = (-\sin \varphi \cos \theta, \cos \varphi \cos \theta, -\sin \theta) \), where \( \varphi \) and \( \theta \) are the angles of deviation from the initial direction of the director. Then the linearized equilibrium equations (2) for perturbations of the angles \( \varphi \) and \( \theta \), which were obtained analogously in [15] for another initial state of the director, can be written in the form

\[
K_{22} \theta_{xx} + K_{11} \theta_{zz} = (K_{22} - K_{11}) \varphi_{xz}
\] (5)

\[
K_{11} \varphi_{xx} + K_{22} \varphi_{zz} = (K_{22} - K_{11}) \theta_{xz}
\] (6)

We will not take into account the boundary perturbations, thus the boundary conditions (3) can be reduced to the relations at \( z = \pm h \) [16]

\[
K_{22} \varphi_z = \theta_z (K_{22} - K_{24})
\] (7)

\[
K_{11} \theta_z = W \theta = \varphi_z (K_{24} - K_{11})
\] (8)

Condition (7) can be applied to both boundaries. In condition (8) the upper and lower signs relate to upper and lower boundaries, respectively.

3. Nontrivial periodic solutions for perturbations

Without loss of generality we will seek the solutions of equations (5), (6) in the form: \( \theta = f(z) \sin k x \), \( \varphi = g(z) \cos k x \). As a result of calculations these one can be written as follows

\[
\theta = \left[ (A_1 + A_2 z) \exp(kz) + (A_3 + A_4 z) \exp(-kz) \right] \sin k x
\]

\[
\varphi = \left[ (B_1 + B_2 z) \exp(kz) + (B_3 + B_4 z) \exp(-kz) \right] \cos k x
\]

where \( A_i \), \( B_j \) are constant. By virtue of (5), (6), they are connected by the relations

\[
B_2 = A_2, \quad k B_1 - k A_1 = \lambda B_2, \quad B_4 + A_4 = 0
\] (9)
\[ kB_3 - kA_3 = \lambda A_4, \quad \lambda = \frac{K_{11} + K_{22}}{K_{11} - K_{22}} \]  

(10)

The boundary conditions (7), (8) together with the relations (9) and (10) make it possible to write a linear homogeneous system for the coefficients \( A_i \) and \( B_i \). The nontrivial solutions for perturbations exist if its determinant is equal to zero. As a result we receive the equations

\[ \pm 2 \left( \frac{1}{K_{11}} - \frac{1}{K_{22}} \right) hK_{22}^2 k^2 + 2W(ch(2kh) \pm 1) = kK_{24} \left( \frac{1}{K_{11}} + \frac{1}{K_{22}} \right) - 4 \) sh(2kh) \]  

(11)

which permit us to find the wave number \( k \) as function of \( K_{ii}, W \) and \( h \).

We will determine that NLC film is unstable if solutions of (11) exist for \( k > 0 \). If \( K_{24} = 0 \), positive \( k \) as root of (11) does not exist and film is stable. As a result of analysis of equation (11) then \( K_{24} \neq 0 \) we can distinguish three domain of splay-bend constant value (all calculations below are made for MBBA parameters, then \( K_{11} = 6 \) pN, \( K_{22} = 4 \) pN and \( W = 4 \cdot 10^{-5} \) N/m if it is not specified separately), which are corresponding to the Ericksen inequalities.

1) When \( 0 \leq K_{24} \leq 2K_{11} \) and \( 0 \leq K_{24} \leq 2K_{22} \) or Ericksen’s inequalities for \( K_{24} \) are satisfied and \( F_V \geq 0 \). In this case positive solutions \( k = k(h) \) in (11) are absent and NLC film is stable.

2) When \( 2K_{22} < K_{24} < 2K_{11} \). In this case we can find positive solutions \( k(h) \), orientational instability appears. But for some value of \( K_{24} \) in this zone function \( k(h) \) is defined only for \( h \), which is less than certain critical value \( h_0 \). Also \( h_0 \) is small and orientational instability exists in very thin films. This result is well compatible with experiments in work [17]. On the Fig. 1 the graph for period \( L = 2\pi/k \) of received solutions as function of film thickness \( 2h \) is shown. Calculations are made for \( K_{24} = 8.8 \) pN. Graph on the Fig. 2 \((K_{24} = 10 \) pN) shows the transition state from the instability in the thin film only to one in the film of arbitrary thickness. Also for this \( K_{24} \) value solutions of (11) coincide if \( 2h > 0.2 \mu m \).

3) If \( K_{24} > 2K_{22} \) and \( K_{24} \geq 2K_{11} \) function \( k(h) \) is defined for the films with arbitrary thickness. On the Fig. 3 the graph for \( L(2h) \) is shown. Calculations are made for \( K_{24} = 14 \) pN. We can see, that two solutions of equation (11) coincide for \( 2h > 3 \mu m \).

Also we need to emphasize that only domain 1 for \( K_{24} \) can be found precisely, because it is determined by condition, that \( F_V \) is positive definite function, only. Properties of solutions in domains 2 and 3 also depend from the anchoring coefficient \( W \). On the Fig. 4 we demonstrate this fact. There are period \( L \) as function of \( K_{24} \) for some values of \( W \) is shown for typical experimental size of NLC films and layers. One can see on this graph, for \( 2h = 10 \div 500 \mu m \) period \( L \) practically does not depend from film thickness. Both solutions of (11) in this case coincide in the investigated range of \( 2h \) similarly previous values of surfacelike constant.

Also if \( W = 0 \) period \( L \) is linear function of \( 2h \) and orientational instability exists for \( K_{24} = 8 \div 12 \) pN. Thus, if anchoring is absent, director field instability appears in case 2 only. Measurements of the splay-bend elastic constant in [5] give us that \( K_{24} \) can fall outside the specified limits and this type of the director instability is rarely observed for shear flows, when we can assume the zero anchoring on the NLC layer boundary [18–20].

4. Conclusions

In the presented work we investigate orientational instability in the NLC films with undisturbed homogeneous plane orientation of director. If we take into account divergent part in the Frank energy and the \( K_{24} \) constant is rather great, orientational instability in the nematic film is possible. This effect appears in the nontrivial periodical solutions, which exist under the action of uniform external forces and boundary conditions. Also this type of instability is occur if Ericksen inequalities for splay-bend constant are not fulfilled.

In case of orientational instability two possibilities exist. In the first one very thin films are instable only, in the second orientational instability does not depend on the film thickness. It is shown relation between two types of instabilities and Ericksen inequalities.
Figure 1. Period $L$ as function of film thickness, case 2, $K_{24} = 8.8 \text{ pN}$.

Figure 2. Period $L$ as function of film thickness $2h$, transition from case 2 to 3, $K_{24} = 10 \text{ pN}$.

Figure 3. Period $L$ as function of film thickness $2h$, case 3, $K_{24} = 14 \text{ pN}$.

Figure 4. Period $L$ as function of film thickness $2h$, case 3. Lines A and C are constructed for $K_{24} = 12 \text{ pN}$, B and D – for $K_{24} = 14 \text{ pN}$; lines A and B are constructed for $W = 40 \mu\text{N/m}$, C and D – for $W = 8 \mu\text{N/m}$.

In addition we analyze how the period of the received nontrivial periodical solutions depends on the anchoring coefficient. It is shown that for zero anchoring instability exists if splay-bend constant is bounded above and below.

This model of director field instability permit us to explain some experimental facts. Also we can calculate relation between period of received periodical solutions and film thickness. This function can be used for splay-bend constant $K_{24}$ measurement.
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