Flexoelectric instability and a spontaneous chiral-symmetry breaking in a nematic liquid crystal cell with asymmetric boundary conditions

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Using both numerical simulations and an approximate analytical theory we describe a flexoelectric-induced instability in a thin nematic liquid crystal layer with asymmetric boundary conditions subjected to an applied electric field. The dependence of the threshold value of the electric field on principal material parameters of the nematic liquid crystal and the director distribution in different regions of the cell have been studied in detail numerically. The results have been compared with a simple analytical theory that enables us to obtain explicit expressions for the threshold electric field and the period of modulation above the threshold. It has been found that in the hybrid aligned nematic cell with homeotropic anchoring on one surface and planar homogeneous anchoring on the other surface, a periodic flexoelectric-induced domain structure appears, above a critical threshold, with a chiral director distribution. The director rotates about the alignment axis when moving along a perpendicular direction in the plane of the cell. The absolute value of the threshold field has been found to depend on the direction of the field due to the initial symmetry of the hybrid aligned cell and the presence of flexoelectricity.

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I. INTRODUCTION

Liquid-crystal materials exhibit a number of instabilities leading to the formation of various periodic structures which are of general interest from a scientific point of view. Periodic structures in thin liquid crystal cells have also attracted significant attention because they can be used in various electro-optic devices and, in particular, as a convenient media for lasing. So far, however, lasing has been achieved either in cholesteric or ferroelectric liquid crystals which possess a natural periodic helicoidal distribution of the molecular orientation, or in nematic liquid crystal cells with prescribed periodic patterns on the surface [1,2]. A disadvantage of the periodically patterned surfaces is related to the restriction to a fixed periodicity which cannot be tuned. In principle, it would be more advantageous to find a system where a periodic structure appears spontaneously, and where the period can be controlled by external factors such as an applied electric field. Perhaps the most well-known periodic instability in liquid crystals caused by an electric field is the formation of Williams domains [3]. The nature of Williams domains is related to electrohydrodynamics, the spacially periodic distribution of the nematic director is induced by the flow of the liquid crystal. Alternatively, electric fields may also induce so-called "flexoelectric domains" which exist in the absence of flow [4–7]. Flexoelectric domains were first observed by Vistin [8] but it took half a decade before it was shown theoretically by Bobylev and Pikin [4] and experimentally by Barnik *et al.* [5,6] that the formation of these domains is related to the flexoelectric effect.

It is interesting to note that before the work of Bobylev and Pikin, Meyer had predicted another electric field induced instability in nematic liquid crystals [9] which is also determined by flexoelectricity. This instability has been predicted to occur in a bulk nematic sample, while the flexoelectric domains described by Bobylev and Pikin can only be stable in thin nematic cells with sufficiently strong surface anchoring. As far as we know, the Meyer instability has never been observed experimentally. In particular, in the experimental studies of Barnik *et al.* [5,6] the periodic structure has been found to appear in the direction perpendicular to the undisturbed director alignment, in agreement with the predictions of [7], while in the Meyer model the periodicity should appear along the alignment direction. It is clear that the confinement effect and the anchoring at the surfaces play a crucial role in the formation of flexoelectric domains in real liquid crystals. Recently an intermediate case has also been considered by Barbero and Lelidis who have studied the flexoelectric instability in a nematic cell in the case of weak boundary conditions.

The theoretical analysis of the flexoelectric instability has largely been restricted to the case of a planar homogeneously aligned nematic cell [4,7,10], with the exception of [11] where the asymmetric boundary conditions have also been considered in the limiting case of weak anchoring. A simple analytical theory has been developed to determine the threshold characteristics of the cell [4] and the approximate director distribution in the limiting case of very strong field [10]. However, the detailed director distribution above the threshold remains unknown. In this paper we consider a flexoelectric instability in a nematic cell with an inhomogeneous distribution of the director in the direction through the cell using both numerical simulation and an approximate analytical approach. In particular, we consider the so-called "hybrid aligned" nematic liquid crystal cell with homeotropic alignment at one surface and planar homogeneous alignment at the other. In a hybrid aligned nematic cell the director configuration has polar symmetry and it is known that such cells possess linear electro-optic properties determined by the

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nonzero flexoelectric polarization within the cell. The influence of this polarity on the nature of the flexoelectric instability is also one of the objectives of this study. Another objective is to determine the three-dimensional director distribution inside the cell above the threshold value of the applied electric field. We will show that the domain structure is characterized by a helical distribution of the director about the alignment axis. In the following section we first perform a detailed numerical study of the flexoelectric instability in a hybrid aligned nematic cell and determine the dependence of the threshold voltage on the ratio of elastic constants of the nematic and on the anisotropy of the flexoelectric coefficients. We then develop a simple analytical theory of the flexoelectric instability which enables us to obtain an explicit expression for the threshold voltage and the period of the domains. Finally we discuss the degree of agreement between the approximate analytical theory and the numerical calculations and summarize the general properties of the flexoelectric instability in a nematic cell with asymmetric boundary conditions.

II. BASIS OF THE NUMERICAL SIMULATION

We have performed a numerical simulation of the director distribution in a hybrid aligned nematic liquid crystal cell of thickness d. The first boundary of the cell, with planar homogeneous director alignment, is located in the plane $z=0$. The alignment direction is parallel to the x-axis, and thus the director at this surface is expressed as $\mathbf{n}=(1,0,0)$. The second boundary, with homeotropic director alignment, is located in the plane $z=d$, and at this surface the director is $\mathbf{n}=(0,0,1)$. The flexoelectric instability has been simulated using the continuum elasticity theory of nematic liquid crystals [12]. Taking into account a contribution from the electric field in the medium, the free energy density of the nonchiral nematic liquid crystal phase can be written in the form

$$F=\frac{1}{2}\{K_{11}(\nabla\cdot\mathbf{n})^2+K_{22}(\mathbf{n}\cdot\nabla\times\mathbf{n})^2+K_{33}(\mathbf{n}\times\nabla\times\mathbf{n})^2+K_{24}\nabla\cdot[(\mathbf{n}\cdot\nabla)\mathbf{n}-(\nabla\cdot\mathbf{n})\mathbf{n}]\}-(\mathbf{E}\cdot\mathbf{P}_f)-\frac{1}{2}(\boldsymbol{\epsilon}\cdot\mathbf{E})\cdot\mathbf{E}, \tag{1}$$

where K_{11}, K_{22}, K_{33}, and K_{24} are the elastic constants which correspond to splay, twist, bend, and saddle-splay deformations, respectively. Here $\mathbf{E}$ is the electric field in the dielectric medium and, in the laboratory frame (x,y,z), the dielectric susceptibility tensor $\boldsymbol{\epsilon}$ can be expressed as $\epsilon_{ij}=\epsilon_\perp\delta_{ij}+(\epsilon_\parallel-\epsilon_\perp)n_in_j$, where $i,j=x,y,z$, and where $\epsilon_\perp$ and $\epsilon_\parallel$ are the transverse and longitudinal (along the director) dielectric permittivities of the nematic phase, respectively. The flexoelectric polarization $\mathbf{P}_f$ can be expressed as

$$\mathbf{P}_f=e_1(\nabla\cdot\mathbf{n})\mathbf{n}-e_3(\mathbf{n}\times\nabla\times\mathbf{n}), \tag{2}$$

where e_1 and e_3 are the flexoelectric coefficients. The displacement field $\mathbf{D}$ can therefore be expressed as

$$\mathbf{D}=\boldsymbol{\epsilon}\cdot\mathbf{E}+\mathbf{P}_f. \tag{3}$$

The governing equations for the nematic director configuration are then found from the classic Ericksen-Leslie theory, where we have assumed that flow is not important in this pattern formation process:

$$-\frac{\partial(F+g)}{\partial n_i}+\frac{\partial}{\partial x}\left(\frac{\partial(F+g)}{\partial n_i/\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{\partial(F+g)}{\partial n_i/\partial y}\right)+\frac{\partial}{\partial z}\left(\frac{\partial(F+g)}{\partial n_i/\partial z}\right)=\gamma_1\frac{\partial n_i}{\partial t}, \tag{4}$$

where $g=\lambda(1-\mathbf{n}^2)/2$, and where λ is a Lagrange multiplier which accounts for the constraint $|\mathbf{n}|=1$. Equation (4) represents a balance between the elastic torque in the left-hand side of the equations and the viscous torque in the right-hand side, where γ_1 is the rotational viscosity of the nematic phase. In the equilibrium state the viscous torque vanishes and the equations are reduced to the Euler-Lagrange equations which are obtained by minimization of the free energy of the nematic layer. These equations are coupled to the governing equation for the electric field distribution within the liquid crystal which, in this nonconducting medium, is Maxwell's equations for the electric field and displacement fields, $\nabla\times\mathbf{E}=0$ and $\nabla\cdot\mathbf{D}=0$. The director and electric field solutions are found using a numerical software package developed by one of the authors [13].

III. RESULTS OF NUMERICAL SIMULATIONS

In this section we present the results of our numerical simulation of the flexoelectric instability in a hybrid aligned nematic cell. The applied electric field is parallel to the z-axis which is normal to surfaces of the cell and the x-axis is parallel to the alignment direction on the surface with planar homogeneous anchoring. At sufficiently low values of the

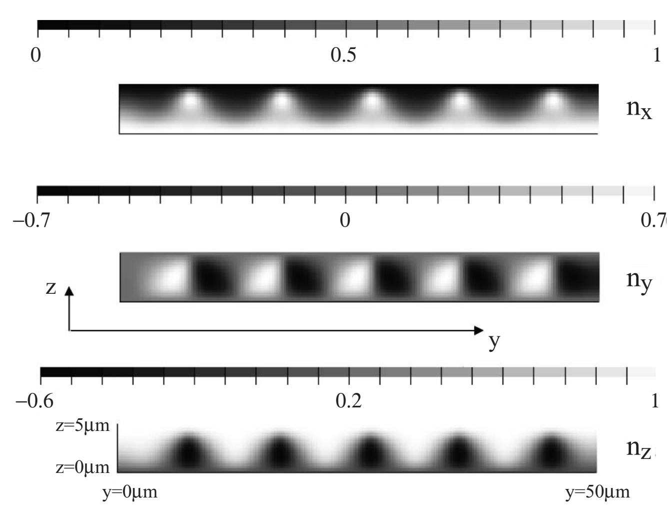

FIG. 1. Periodic distribution of the components of the nematic director $\mathbf{n}$ in the hybrid aligned nematic liquid crystal cell above the threshold at $U=10$ V. Rulers above each plot provide the grayscale values and the parameters used are $d=5$ μm, $K_{11}=6$ pN, $K_{22}=3$ pN, $K_{33}=10$ pN, $e_1=10$ pC/m, $e_3=0$, and $\Delta\epsilon=0$.

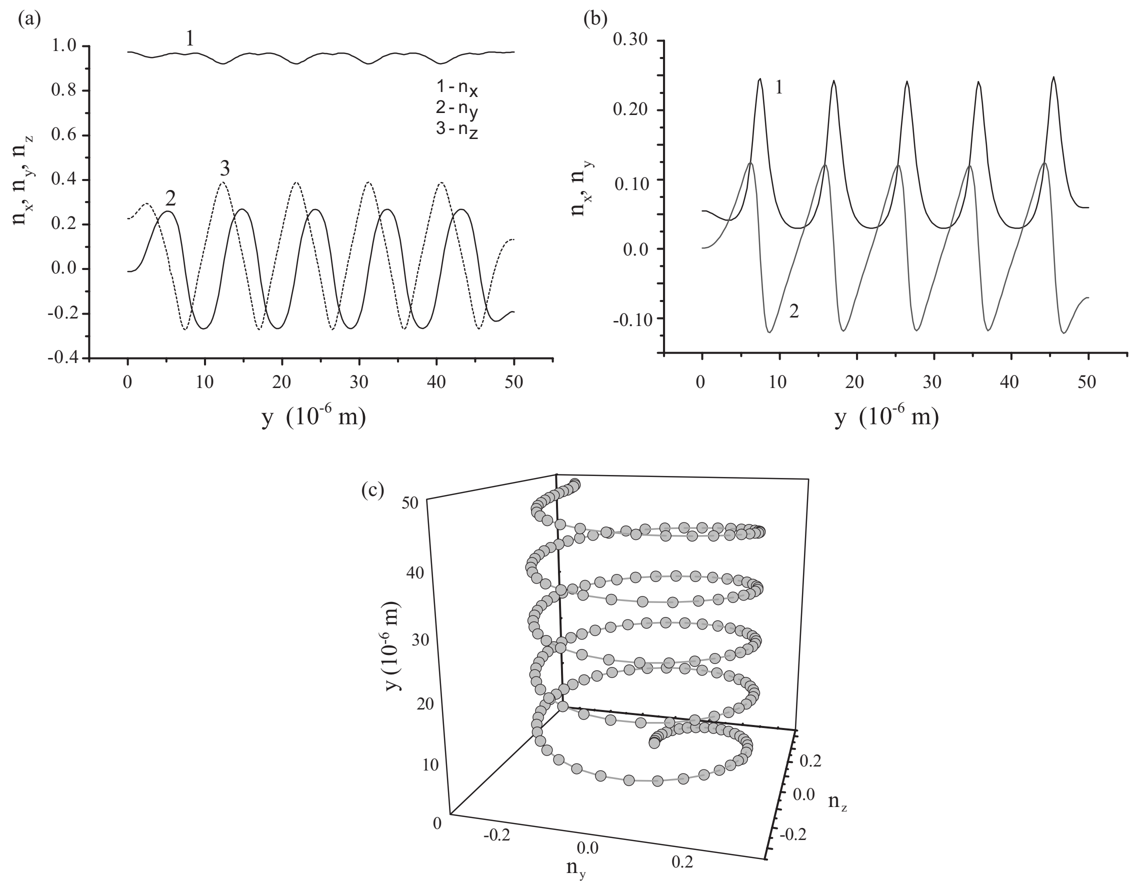

FIG. 2. Variation of the director components n_y and n_z along the y-axis: (a) at a distance of 0.5 μm from the surface with planar alignment; (b) at a distance of 0.5 μm from the surface with homeotropic alignment; (c) the y and z components of the director are plotted as y varies to show the chiral nature of the distortion. Parameter values are the same as in Fig. 1.

electric field the director distribution in the cell is homogeneous in the x,y plane and the director $\mathbf{n}$ depends only on z. The angle $\theta(z)$ between the director and the z-axis changes gradually from $\theta=0$ at the surface with planar anchoring to $\theta=\pi/2$ at the surface with homeotropic anchoring, the standard director distribution in the hybrid aligned nematic cell (see, for example, [14]). However, for higher electric field strengths the calculated director distribution is presented in Fig. 1. There is clearly a spacial periodicity of the director distribution along the y-axis, i.e., in the direction perpendicular to the initial director orientation on the surface with planar anchoring. The periodicity of the director distribution appears when the applied voltage exceeds a threshold value. The simulations show that the periodic director distribution evolves continuously starting from an extremely small amplitude of the director modulation at the threshold, $\delta n_z \sim 10^{-8}$ which is of the order of the typical numerical error of the system. The results presented in Fig. 1 correspond to a nematic liquid crystal with typical values of the elastic constants ($K_{11}=6$ pN, $K_{22}=3$ pN, $K_{33}=10$ pN, and $K_{24}=0$) and zero dielectric anisotropy ($\epsilon_\perp=\epsilon_\parallel$). In this case the threshold voltage is found to be about 9 V for a nematic cell of thickness $d=5$ μm. In Fig. 2 we show the periodic director distribution in the plane $z=0.5$ μm which is close to the surface with planar homogeneous anchoring [Fig. 2(a)], and in the plane $z=4.5$ μm which is close to the surface with homeotropic anchoring [Fig. 2(b)]. One can readily see from Fig. 2 that at $U=10$ V, i.e., about 1 V above the threshold value, the director distribution is periodic along the y-axis, and thus it differs qualitatively from the initial one-dimensional (1D) distribution below the threshold. Close to the surface with homogeneous alignment the component of the director n_x is nearly constant while the components n_z and n_y change periodically with the same period but with a phase shift of $\pi/2$. Neglecting the higher harmonics, the components of the director can be expressed as

$$n_x \approx \text{const}; \quad n_y \approx n_y^0 \cos(ky+\delta); \quad n_z \approx n_z^0 \sin(ky+\delta); \tag{5}$$

where δ is a constant phase and where the phase shift between n_y and n_z is equal to $\pi/2$. Thus the projection of the director on the (z,y) plane, $\mathbf{n}_\perp=(n_y,n_z)$, rotates about the x-axis while moving along the y-axis. This periodicity of $\mathbf{n}_\perp$ is shown in the lower part of Fig. 2(a). Note that such a "rotating" director distribution appears also in the case of the planar homogeneously aligned nematic liquid crystal cell. It is also interesting to note that the director distribution described by Eq. (5) is chiral because the pseudoscalar quantity $(\mathbf{n}\cdot\nabla\times\mathbf{n})\neq 0$. However, the initial configuration below the threshold is achiral, and thus chiral flexoelectric domains appear as a result of the chiral-symmetry breaking.

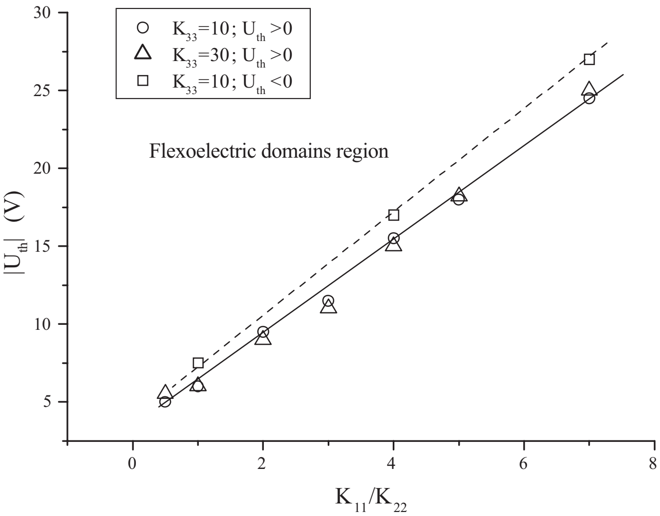

FIG. 3. Dependence of the threshold voltage on the ratio of elastic constants K_{11}/K_{22} when $e_1=10$ pC/m, $e_3=0$, and for different directions of the electric field: upper curve (squares) for negative voltages and lower curve (triangles and circles) for positive voltages. For positive voltages two different values of $K_{33}=10$ pN (triangles) and $K_{33}=30$ pN (circles) have been used. Other relevant parameters are $d=5$ μm and $\Delta\epsilon=0$.

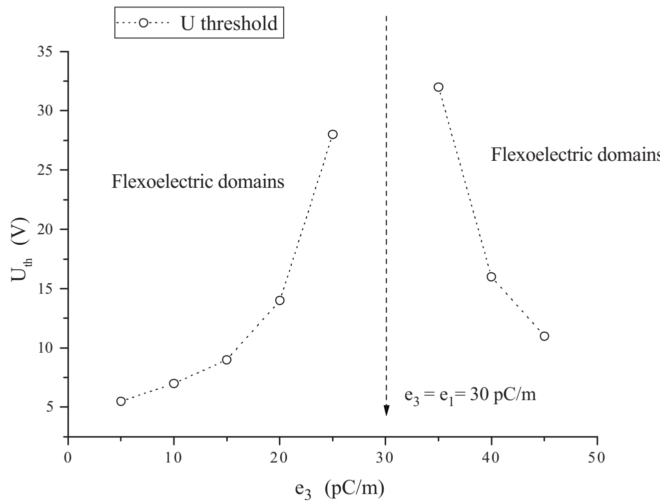

FIG. 4. Dependence of the threshold voltage on the difference of flexoelectric coefficients $\Delta e=e_1-e_3$ for fixed $e_1=30$ pC/m and for parameter values $d=5$ μm, $K_{11}=6$ pN, $K_{22}=3$ pN, $K_{33}=10$ pN, and $\Delta\epsilon=0$.

Numerical simulations indicate that the periodicity along the y-axis depends both on the applied voltage and on the thickness d of the nematic liquid crystal cell. It is interesting that just above the threshold voltage the period of the domain structure is approximately equal to double the value of the nematic layer thickness d, i.e., the wave vector k of the field induced periodic structure is given by

$$k \approx \left. \frac{\pi}{d} \right|_{U \approx U_{th}}. \tag{6}$$

This result is in agreement with the estimates made in [4] for the planar homogeneously aligned nematic cell. Upon increasing the applied electric field the wave vector k decreases, but this dependence appears to be strongly nonlinear.

Close to the surface with homeotropic anchoring the director distribution is more complex [see Fig. 2(b)] because of the strong variation of the n_x component. A contribution from higher harmonics is also larger in this region. However, in this region one also finds some rotation of the director around the x-axis while moving along the y-axis [see Fig. 2(c)].

Dependence of the threshold voltage on the elastic constants of the nematic is presented in Fig. 3. The values of the threshold voltage have been obtained in the following way. From a voltage above the threshold the voltage was decreased gradually until the periodic domains disappear. The minimum voltage for which stable domains occur was considered to be the threshold. One can readily see from Fig. 3 that when $e_3=0$ and for fixed K_{22} the threshold voltage depends explicitly on K_{11} and does not depend on K_{33}. This implies that in this particular case ($e_3=0$) the periodic director distribution first appears in the region close to the surface with planar homogeneous alignment. From Fig. 3 we see that the threshold voltage increases linearly with increasing K_{11} and both the threshold voltage and the slope of the linear dependence in Fig. 3 depend on the sign of the applied electric field. From the general point of view this is related to the polar symmetry of a hybrid aligned nematic cell which possesses a nonzero flexoelectric polarization across the cell. However, this particular result is nontrivial because the sensitivity to the sign of the field is preserved even at zero dielectric anisotropy. Indeed, in the case of a homogeneous electric field one can readily show that the average coupling between the field and the flexoelectric polarization, described by the integral $\int_0^d EP_f dz$ reduces to a surface constant term in the case of strong anchoring on both surfaces of the hybrid aligned nematic cell. However, this result is no longer valid in the case of an inhomogeneous director distribution. Thus in the presence of the flexoelectric domains the flexoelectric coupling results in an additional torque acting on the nematic director. As a result, the flexoelectric domains disappear at a different absolute value of the applied electric field, depending on its sign. The dependence on the sign of the electric field can be more pronounced in the case of nonzero dielectric anisotropy which enhances the inhomogeneous electric field distribution. It is also worth noting that, due to the symmetry of the flexoelectric contribution, pitch of the chiral rotation of the director also changes sign (left-handed rotation or right-handed rotation) when the electric field changes sign.

In the case of a nonzero bend flexoelectric coefficient $e_3 \neq 0$ the threshold voltage depends on the difference $e_1 - e_3$ and diverges at $e_1=e_3$ as shown in Fig. 4. One can readily see that the threshold voltage is sensitive to the sign of e_1-e_3 because the curves in Fig. 4 are not symmetric about $e_1=e_3$. In the following section we discuss all the qualitative properties of the threshold electric field using the results of a simplified analytical theory.

IV. ANALYTICAL APPROACH

In the hybrid aligned nematic liquid crystal cell the director distribution is always inhomogeneous, and as a result there exists a distribution of the flexoelectric polarization which is proportional to the gradient of the director [see Eq. (2)]. This polarization distribution creates an inhomogeneous electric field, and therefore the electric field at a given point inside the cell may differ from the applied field. This local field effect has been taken into account explicitly in the numerical simulations described in the previous two sections where no approximations have been made. In this section we develop a simple analytical theory of the flexoelectric instability in a hybrid aligned cell assuming that the local electric field inside the cell is equal to the applied field. With this simplification it is possible to obtain explicit analytical expressions for the threshold field which can be compared with the results of numerical simulations. The free energy density of the hybrid aligned nematic cell is given in Eq. (1); where the electric field $\mathbf{E}$ is now assumed to be constant and parallel to the z-axis which is perpendicular to the flat surfaces of the cell. In the case of infinite anchoring boundary conditions on both surfaces of the hybrid aligned nematic cell, the director $\mathbf{n}(x,y,z)$ can be written as $\mathbf{n}(z=0)=(1,0,0)$ and $\mathbf{n}(z=d)=(0,0,1)$ for all x and y.

Let us consider first the director distribution in the hybrid aligned nematic cell without an external field. In such a cell the director is parallel to the (x,z) plane, and its components can be expressed in terms of the angle Θ between the director and the x-axis:

$$n_x = \cos \Theta(z); \quad n_y = 0; \quad n_z = \sin \Theta(z). \tag{7}$$

It is well-known that for this case and when $K_{11}=K_{33}$ the distortion free energy density of the nematic [the first four terms in Eq. (1)] is reduced to $\frac{1}{2}K(\frac{d\Theta}{dz})^2$. Minimization of this free energy results in a linear dependence of Θ on z. Taking into account the boundary conditions one obtains $\Theta = \pi z/2d$.

Slightly above the threshold the director can be expressed as

$$\mathbf{n} = \mathbf{n}_0 + \delta\mathbf{n}, \tag{8}$$

where $\mathbf{n}_0$ is the unperturbed director given by Eq. (9), and $\delta\mathbf{n}$ is a small deviation. Taking into account that in the first approximation the small deviation $\delta\mathbf{n}$ must be perpendicular to $\mathbf{n}_0$, i.e., $(\mathbf{n}_0\cdot\delta\mathbf{n})=0$, the vector $\delta\mathbf{n}$ can be expressed in terms of two unknown functions $n_1(y,z)$ and $n_2(y,z)$:

$$\delta\mathbf{n} = [-n_2(y,z)\sin \Theta(z), \quad n_1(y,z), \quad n_2(y,z)\cos \Theta(z)], \tag{9}$$

where $n_1,n_2 \ll 1$. Here we have taken into account that according to the results of numerical simulation the director does not depend on x and thus the functions n_1 and n_2 depend only on y and z. Finally $\delta\mathbf{n}=0$ on both surfaces of the cell because the anchoring is assumed to be infinite and thus the orientation of the director is fixed at the surfaces. If we consider periodic instabilities of the unperturbed director configuration, the functions $n_1(y,z)$ and $n_2(y,z)$ are periodic functions of y and must vanish at the surfaces $z=0$ and $z=d$. In a first mode approximation they can be written in the form

$$n_1(y,z) = N_1 \sin\left(\frac{\pi z}{d}\right)\cos(ky),$$

$$n_2(y,z) = N_2 \sin\left(\frac{\pi z}{d}\right)\sin(ky), \tag{10}$$

where we have taken into account that the phase shift in the y direction between the director components $\delta n_z = n_2(y,z)\cos \Theta(z)$ and $\delta n_y = n_1(y,z)$ should be equal to $\pi/2$ according to the results of numerical simulations discussed above. The dependence of n_1 and n_2 on z in Eq. (10) is supported by numerical simulations as shown in Fig. 1. Substituting Eq. (10) into Eq. (9) and then into Eq. (8) one obtains the following expression for the perturbed director above the threshold in terms of two unknown amplitudes N_1 and N_2:

$$n_x = \cos \Theta(z) - N_2 \sin\left(\frac{\pi z}{d}\right)\sin(ky)\sin \Theta(z),$$

$$n_y = N_1 \sin\left(\frac{\pi z}{d}\right)\cos(ky),$$

$$n_z = \sin \Theta(z) + N_2 \sin\left(\frac{\pi z}{d}\right)\sin(ky)\cos \Theta(z). \tag{11}$$

Equation (11) is now substituted into the following equation for the total free energy per unit area of the hybrid aligned nematic cell:

$$\mathcal{F} = \frac{k}{2\pi}\int_0^{2\pi/k}\left(\int_0^d F dz\right)dy, \tag{12}$$

where the free energy density F is given by Eq. (1). Minimization of the total free energy (12) with respect to N_1 and N_2 and, since perturbations are small, considering only leading order terms in N_1 and N_2, yields the following system of two simultaneous equations for N_1 and N_2, which may easily be obtained using a software package such as MAPLE:

$$N_1\pi[\alpha_1 K_{11}(dk)^2 + \pi^2(\alpha_2 K_{22} + \alpha_3 K_{11})] + N_2(dk)[\alpha_4 \Delta e(dE) + \alpha_5 \pi(K_{11} - K_{22})] = 0;$$

$$N_1(dk)[\alpha_4 \Delta e(dE) + \alpha_5 \pi(K_{11} - K_{22})] + N_2\pi[\alpha_1 K_{22}(dk)^2 + \alpha_6 \pi^2 K_{11} - \alpha_3 \epsilon_0 \Delta\epsilon(dE)^2] = 0, \tag{13}$$

where $\Delta e = e_1 - e_3$ and the numerical coefficients $\alpha_1=120$, $\alpha_2=75$, $\alpha_3=60$, $\alpha_4=256$, $\alpha_5=192$, and $\alpha_6=165$ appear after integration of various trigonometric functions which describe perturbations with respect to the inhomogeneous director distribution in the hybrid aligned cell. Equations (13) have nontrivial solutions ($N_1 \neq 0$, $N_2 \neq 0$) only if the determinant of this system of equations is equal to zero. This condition produces an equation for the threshold electric field in terms of the wave vector k which can be written in the form of a quadratic equation,

$$\beta_1 E^2 + \beta_2 E + \beta_3 = 0, \tag{14}$$

where

$$\beta_1 = d^2\{\epsilon_0 \Delta\epsilon \alpha_3 \pi^2 [\pi^2(\alpha_2 K_{22} + \alpha_3 K_{11}) + (kd)^2 \alpha_1 K_{11}] - (kd)^2 \alpha_4{}^2 (\Delta e)^2\}, \tag{15}$$

$$\beta_2 = 2\pi d \alpha_4 \alpha_5 (kd)^2 (K_{22} - K_{11}) \Delta e, \tag{16}$$

$$\beta_3 = \pi^2[\alpha_1 K_{11}(kd)^2 + \pi^2(\alpha_2 K_{22} + \alpha_3 K_{11})][\alpha_1 K_{22}(kd)^2 + \alpha_6 \pi^2 K_{11}] - (kd)^2 \alpha_5^2 \pi^2 (K_{11} - K_{22})^2. \tag{17}$$

Equation (14) has two solutions for the threshold voltages, which are related to the threshold fields by $U_{th}=E_{th}d$,

$$U_{th}^{(+)} = \frac{d}{2}\left(-\frac{\beta_2}{\beta_1} + \sqrt{\left(\frac{\beta_2}{\beta_1}\right)^2 - 4\frac{\beta_3}{\beta_1}}\right), \tag{18}$$

$$U_{th}^{(-)} = \frac{d}{2}\left(-\frac{\beta_2}{\beta_1} - \sqrt{\left(\frac{\beta_2}{\beta_1}\right)^2 - 4\frac{\beta_3}{\beta_1}}\right), \tag{19}$$

which correspond to different critical external voltage values, one positive and one negative. Thus the absolute value of the threshold voltage depends on the direction of the field in accordance with the results of numerical simulations. In fact it is clear from Eqs. (18) and (19) that if $\beta_2 \neq 0$ there will always be a difference in the absolute values of positive and negative threshold voltages. If, however, $\Delta e=0$ or $K_{11}=K_{22}$ then $\beta_2=0$ and the absolute threshold voltage value is the same for positive and negative fields. These explicit expressions, Eqs. (18) and (19), for the threshold values of the voltage possess a number of other qualitative properties which can be compared with numerical solutions. For example, according to Eqs. (18) and (19), the threshold voltages do not depend on the bend elastic constant K_{33}. This result is confirmed by numerical simulations (see Fig. 3). In the case of zero dielectric anisotropy ($\Delta\epsilon=0$) the coefficient β_1 is given by $\beta_1=\gamma(\Delta e)^2$. Thus β_1 is proportional to the square of the anisotropy of the flexoelectric coefficients, Δe, and one can readily see from Eqs. (18) and (19) that in his case the threshold voltage diverges when $\Delta e=0$. As discussed in the previous section, this divergence has also been found in numerical simulations for $\Delta\epsilon=0$ (see Fig. 4).

The dependence of the threshold values $U_{th}^{(+)}$ and $U_{th}^{(-)}$ on the ratio of the elastic constants K_{11}/K_{22} is presented in Fig. 5. Comparing Figs. 5 and 3 one concludes that the qualitative behavior of the threshold voltages is well-described by the simple analytical theory. At the same time there is a significant quantitative discrepancy which is mainly determined by the following factors. First, a number of approximations have been made in the simple analytical theory developed in this section. In particular, the unperturbed profile of the angle $\Theta(z)$ in the hybrid aligned cell has been assumed to be linear which is formally valid only if $K_{11}=K_{33}$. We have also neglected the inhomogeneous distribution of the electric field inside the cell. Second, numerical calculations of threshold parameters are not very accurate in general because it is very difficult to determine the exact value of the parameter which corresponds to the appearance of the infinitesimally small periodic perturbation.

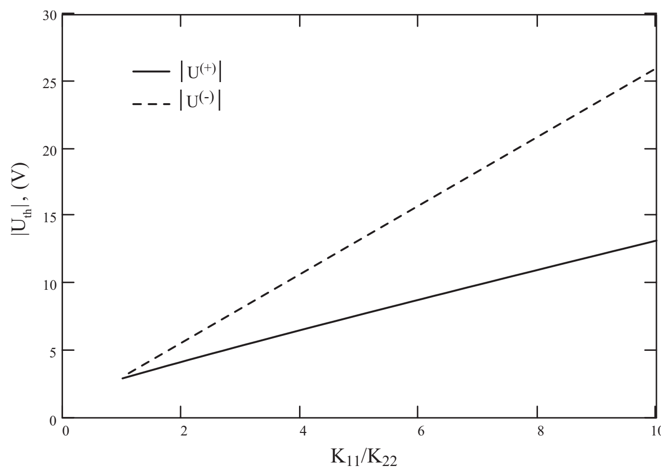

FIG. 5. Dependence of the threshold voltage on the ratio of elastic constants K_{11}/K_{22} for positive (upper curve) and negative directions of the external field, as follows from Eqs. (18) and (19) with parameter values $d=5\ \mu$m, $K_{11}=K_{33}$, $e_1=10$ pC/m, $e_3=0$, and $\Delta\epsilon=0$.

The wave vector k of the periodic director distribution can also be determined by minimization of the threshold voltage as a function of k. In the case of $\Delta\epsilon=0$ only the ratio β_3/β_1 in Eqs. (18) and (19) depends on k. It can therefore be shown that the minimization of the threshold voltage is equivalent to the minimization of the absolute value of the ratio $|\beta_3/\beta_1|$ which can be expressed as

$$|\beta_3/\beta_1| = \delta_1 \frac{1}{k^2} + \delta_2 k^2 + \text{const}, \tag{20}$$

where

$$\delta_1 = -\frac{\pi^6 \alpha_6 K_{11}(\alpha_2 K_{22} + \alpha_3 K_{11})}{d^4 \alpha_4^2 (\Delta e)^2}, \tag{21}$$

$$\delta_2 = \frac{\pi^2 \alpha_1{}^2 K_{11} K_{22}}{\alpha_4{}^4 (\Delta e)^2}. \tag{22}$$

Minimization of Eq. (20) yields the following expression for the wave vector $2\pi/k$:

$$\frac{2\pi}{k} = 2d\left[\frac{55}{64} + \frac{11}{16}\left(\frac{K_{11}}{K_{22}}\right)\right]^{-1/4}. \tag{23}$$

The dependence of the period of the domain structure on the ratio K_{11}/K_{22} is presented in Fig. 6. The period of the flexoelectric domains has the correct order of magnitude, i.e., it is of the order of $2d$, and more specifically when $K_{11}=K_{22}$ the period is $2\pi/k=1.7934d$.

V. DISCUSSION

In this paper we have investigated the appearance of flexoelectric domains in a hybrid aligned nematic liquid

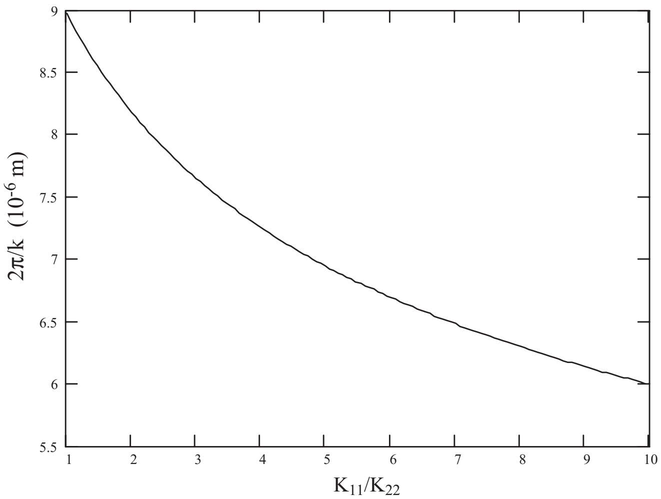

FIG. 6. Dependence of the period of the flexoelectric domain structure on the ratio K_{11}/K_{22} as follows from Eq. (23) for $d=5\ \mu\text{m}$.

crystal cell in an external electric field. The flexoelectric instability induced by the electric field was studied numerically by direct minimization of the free energy accompanied by the full numerical solution of the corresponding electrostatic problem. It has been found that above a certain threshold value of the electric field (or the threshold voltage for a cell of particular thickness) a periodic flexoelectric domain structure appears which is qualitatively similar to the one observed by Barnik *et al.* in the planar homogeneous nematic cell [5,6]. This domain structure is determined by the rotation of the director about the alignment direction (on the surface with planar anchoring) when moving in a perpendicular direction in the plane of the cell. It is interesting to note that this director distribution is chiral and is characterized by a nonzero twist deformation. At the same time the system below the threshold is nonchiral. Indeed, below the threshold electric field the director distribution in the hybrid aligned nematic cell is confined to the (x,z) plane where the x-axis is parallel to the alignment direction and the z-axis is perpendicular to the cell. The external electric field is parallel to the z-axis, and thus the (x,z) plane appears to be a mirror plane of the cell below the threshold. Above the threshold voltage the periodic chiral director distribution appears spontaneously. Such a nematic cell in an external electric field appears, therefore, to be an interesting example of a spontaneous chiral-symmetry breaking. One notes also that, at least close to the boundary with planar anchoring, the twist deformation of the nematic is approximately proportional to $\sin qy$, i.e., the "chirality density" measured by the twist deformation alternates in sign along the y-axis. Another interesting property of the flexoelectric instability studied in this paper is related to the polarity of the hybrid aligned cell which has two nonequivalent surfaces. In such an asymmetric cell the director distribution across the cell is inhomogeneous even without any external field, and therefore there exists a nonzero flexoelectric polarization distribution inside the cell which is linearly coupled to the electric field. As a result the absolute value of the threshold voltage depends on the direction of the external electric field, as shown in Figs. 3 and 5.

Based on the results of the simulations, we have also developed a simple analytical theory of the flexoelectric instability and obtained explicit analytical expressions for the threshold voltage and the period of the flexoelectric domain structure as functions of elastic constants and flexoelectric coefficients of the nematic liquid crystal. The theory does not take into account an inhomogeneous electric field distribution inside the cell (the same approximation has been made in [4,7,10]), but the results are in qualitative agreement with numerical simulations as discussed in detail in Sec. III. In particular, the theory describes the dependence of the threshold voltage on the direction of the electric field inside the asymmetric cell.

This flexoelectric domain structure which may be induced by an external electric field in hybrid nematic liquid crystal cells may be interesting from the point of view of applications. Recently a periodically modulated structure has been induced in a thin nematic cell by a holographic grating recorder on the photopolymer aligning layer [1]. The resulting structure is characterized by enhanced diffraction efficiency and can be used in polarized optical devices. A photoinduced surface grating on a polymer film has also been used in the fabrication of the distributed feedback laser [2]. However, from a practical point of view, aligning surfaces with recorded gratings have several disadvantages. First, the period of modulation cannot be dynamically tuned and, second, the fabrication of such periodic surfaces is a relatively complex and expensive procedure. In contrast, the periodic domain structure induced by an external electric field appears self-consistently in a standard cell. The periodic structure can be turned on and off by switching the applied voltage, and the period can be tuned by increasing the external electric field. Thus the appearance of flexoelectric domains in hybrid nematic liquid crystal cells deserves a detailed experimental study.

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