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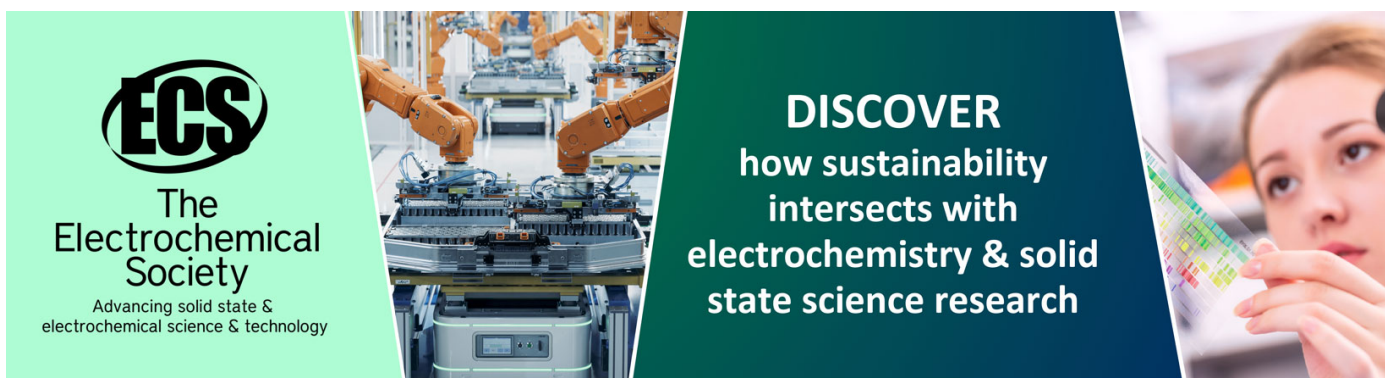
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Effect of flexoelectricity on the Frèedericksz transition in chiral nematics with negative dielectric anisotropy

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Abstract. It is shown theoretically that due to the flexoelectric effect the electric field driven Frèedericksz transition can take place in chiral nematic (cholesteric) liquid crystal with negative dielectric anisotropy. It is especially noteworthy, since such a transition in a plane parallel cell is impossible in the absence of flexoelectricity. The spatial inhomogeneity of the electric field is taken into account in the free energy alongside with the traditionally considered terms, describing the orientation elasticity and the anchoring at the boundaries. The phase diagrams are plotted and the orientation structures above the threshold are analyzed basing on the free energy minimization. A comparison between the phase diagrams for liquid crystals with positive and negative anisotropy of dielectric permittivity is made. It was found, that for sufficiently high flexoelectric coefficients the orientational structure can be described by simple functions. In this case, as a result of the Frèedericksz transition, the orientation structure of the liquid crystal changes from planar helicoidal to a hybrid one. This gives rise to new opportunities for the design of switching devices.

1. Introduction

The Frèedericksz effect was discovered in the twenties of the 20th century and has been especially intensively investigated in recent decades. This is due to the rapid development of liquid crystal display, switching, and other devices based on the Frèedericksz effect. The essence of the effect lies in the possibility of reorientation of a liquid crystal molecules by small external electric and magnetic fields. Here we study the electric field driven Frèedericksz transition in a plane parallel cholesteric liquid crystal (CLC) cell.

2. CLC Model

We assume that the liquid crystal is enclosed in the region $0 \leq z \leq L$ between two plane electrodes with applied voltage U . The averaged orientation of the molecules is described by a unit vector director $\mathbf{n}$. In the presence of flexoelectricity the electric displacement has the form

$$\mathbf{D} = \hat{\epsilon}\mathbf{E} + 4\pi\mathbf{P}_{\text{flex}}, \quad (1)$$



where $\varepsilon_{\alpha\beta} = \varepsilon_{\perp}\delta_{\alpha\beta} + \varepsilon_a n_{\alpha}n_{\beta}$, $\mathbf{P}_{\text{flex}} = e_1 \mathbf{n} \text{div } \mathbf{n} + e_3 \text{curl } \mathbf{n} \times \mathbf{n}$, $\varepsilon_a = \varepsilon_{\parallel} - \varepsilon_{\perp}$, $\varepsilon_{\parallel}$ and $\varepsilon_{\perp}$ are the dielectric permittivities parallel and perpendicular to $\mathbf{n}$, e_1 and e_3 are the flexoelectric coefficients [1]. The system is assumed to be homogeneous in x, y directions, so $\mathbf{n} = \mathbf{n}(z)$. We parametrize the vector director $\mathbf{n}$ as

$$n_x = \sin \theta \cos \varphi, \quad n_y = \sin \theta \sin \varphi, \quad n_z = \cos \theta, \quad (2)$$

with polar and azimuthal angles θ and φ respectively.

The free energy of CLC cell in terms of θ and φ can be expressed as

$$\mathcal{F} = \frac{S_{\perp}}{2} \left(K_{22} q_0^2 L + \int_0^L \left[A(\theta)(\theta')^2 + B(\theta)(\varphi')^2 - 2C(\theta)\varphi' \right] dz \right. \\ \left. + \sum_{\alpha=1,2} \left[W_{\theta}^{(\alpha)} \sin^2(\theta - \theta_0^{(\alpha)}) + W_{\varphi}^{(\alpha)} \sin^2(\varphi - \varphi_0^{(\alpha)}) \right] - \frac{1}{4\pi} (U - 4\pi\bar{e}J_1)^2 J \right), \quad (3)$$

where the prime denotes the derivative with respect to z , $S_{\perp}$ is the area of the boundary plates,

$$A(\theta) = K_{11} \sin^2 \theta + K_{33} \cos^2 \theta + 4\pi\bar{e}^2 \sin^2 2\theta / \mathcal{E}(\theta), \quad \mathcal{E}(\theta) = \varepsilon_{\perp} + \varepsilon_a \cos^2 \theta, \\ B(\theta) = \sin^2 \theta (K_{22} \sin^2 \theta + K_{33} \cos^2 \theta), \quad C(\theta) = q_0 K_{22} \sin^2 \theta,$$

K_{ii} are the elastic Frank moduli, $\bar{e} = (e_1 + e_3)/2$ is the mean flexoelectric coefficient, π/q_0 is the helix period, $W_{\theta, \varphi}^{(\alpha)} > 0$ are the surface anchoring energy moduli ($\alpha = 1, 2$ correspond to the boundaries $z = 0, L$, respectively), the angles $\theta_0^{(\alpha)}$ and $\varphi_0^{(\alpha)}$ describe the easy directions at the boundaries;

$$J^{-1} = \int_0^L \frac{dz}{\mathcal{E}(\theta)}, \quad J_1 = \varepsilon_a^{-1} \ln \frac{\mathcal{E}(\theta(0))}{\mathcal{E}(\theta(L))}. \quad (4)$$

In the absence of flexoelectricity, $\bar{e} = 0$, the free energy expression (3) is the same as one in [2]. In the case of zero external voltage, $U = 0$, the equilibrium structure has the form $\theta(z) \equiv \pi/2$ and $\varphi(z) = \varphi_0^{(1)} + q_0 z$.

The equilibrium CLC structure obeys functional integro-differential Euler-Lagrange equations,

$$A(\theta)\theta'^2 + B(\theta)\varphi'^2 - (U - 4\pi\bar{e}J_1)^2 J^2 / (4\pi\mathcal{E}(\theta)) = c_1, \quad (5)$$

$$B(\theta)\varphi' - C(\theta) = c_2, \quad (6)$$

and four boundary conditions ($\alpha = 1, 2$)

$$2(-1)^{\alpha} [A(\theta)\theta' + \bar{e} (U - 4\pi\bar{e}J_1) J \sin 2\theta / \mathcal{E}(\theta)] + W_{\theta}^{(\alpha)} \sin 2(\theta - \theta_0^{(\alpha)}) \Big|_{z=l_{\alpha}} = 0, \quad (7)$$

$$2(-1)^{\alpha} (B\varphi' - C) + W_{\varphi}^{(\alpha)} \sin 2(\varphi - \varphi_0^{(\alpha)}) \Big|_{z=l_{\alpha}} = 0. \quad (8)$$

In the Eqs. (5), (6) we carry out the order reduction procedure for the Euler-Lagrange equations, that gives rise to the arbitrary constants $c_{1,2}$.

In order to analyse the CLC equilibrium structure we use the direct method of variational calculus based on the fact that this structure affords a minimum to $\mathcal{F}$. The minimization procedure is organized as follows. We use the trial function for the angle θ in the form

$$\theta(z) = \pi/2 + \delta_1 \frac{\sinh \xi(L-z)}{\sinh \xi L} + \delta_2 \frac{\sinh \xi z}{\sinh \xi L} + \sum_{n=1}^N c_n \sin(\pi n z / L), \quad (9)$$

where $\xi = \sqrt{(K_{33}q_0^2 - \varepsilon_a U^2/(4\pi L^2))} K_{11}^{-1}$ is the characteristic length; δ_1, δ_2 , and the coefficients $c_n, n = 1, \dots, N$ are adjustable parameters. Equations (6), (8) permit one to eliminate variable $\varphi(z)$ from the minimization procedure while the Eq. (7) decrements by two the number of the adjustable parameters. In the last step the Eq. (5) is used to control the quality of the final equilibrium structure. The planar helicoidal structure corresponds to $\delta_{1,2} = 0$ and $c_n = 0$. A distorted “phase” arises when some of the parameters $\delta_{1,2}, c_n$ are nonzero. In what follows we present the results for systems with $\varepsilon_a < 0$ and for more widely investigated systems with $\varepsilon_a > 0$. Note that some issues regarding the Frèedericksz transition in nematic LC cells with flexoelectricity and with positive dielectric anisotropy were investigated in [3, 4]. In what follows we fix the signs $\bar{e} \geq 0$ and $U \geq 0$. Obtained areas of the stability of the planar helicoidal and of the distorted structures in $(\bar{e}, U)$ -plane are shown in Fig. 1. The material constants were taken

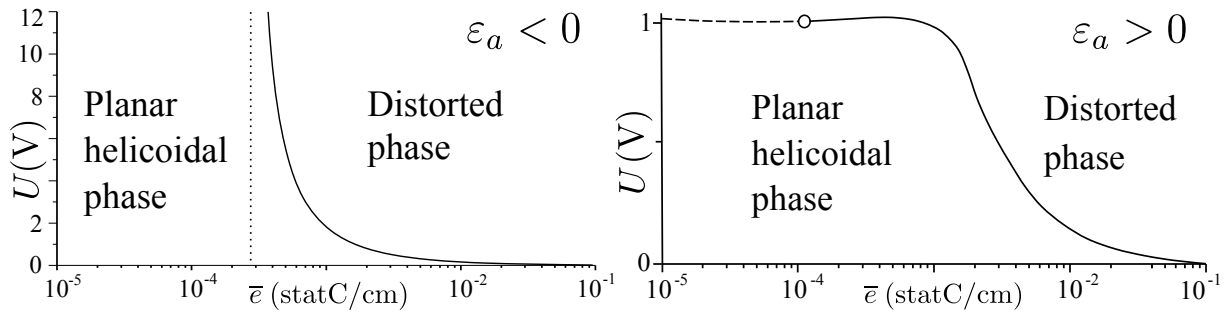


Figure 1. Phase diagram for the cases of $\varepsilon_a < 0$ and $\varepsilon_a > 0$. Line types: — and — — — are the interphase boundaries for continuous and discontinuous transitions respectively; ····· is the asymptote of interphase boundary in the case $\varepsilon_a < 0$, and $\bigcirc$ is the tricritical point.

the same as in Ref. [2]: $K_{11} = 0.42 \times 10^{-6}$ dyn, $K_{22} = 0.23 \times 10^{-6}$ dyn, $K_{33} = 0.53 \times 10^{-6}$ dyn, $q_0 = 500 \text{ cm}^{-1}$, $L = 60 \text{ }\mu\text{m}$, $W_\theta^{(1,2)} = 1.5 \times 10^{-3} \text{ erg/cm}^2$, $W_\varphi^{(1,2)} = 1.5 \times 10^{-4} \text{ erg/cm}^2$, $\varepsilon_\perp = 16.2$, $\varepsilon_\parallel = 7.2$ for $\varepsilon_a < 0$ and $\varepsilon_\perp = 7.2$, $\varepsilon_\parallel = 16.2$ for $\varepsilon_a > 0$. The parameters q_0 and L correspond to the super-twisted LC cell with $q_0 L = 3$. In Fig. 1 one can see quite a surprising result for $\varepsilon_a < 0$. It turns out that there exists a value of $\bar{e}$ (the vertical asymptote) above which the distorted structure can exist. Below this limit value the distorted phase does not exist for arbitrary U . The profiles of polar angle $\theta(z)$ calculated for fixed voltage $U = 1.2 \text{ V}$ and different $\bar{e}$ are shown in Fig. 2. When $\bar{e}$ is rather small the CLC structures are sufficiently different for

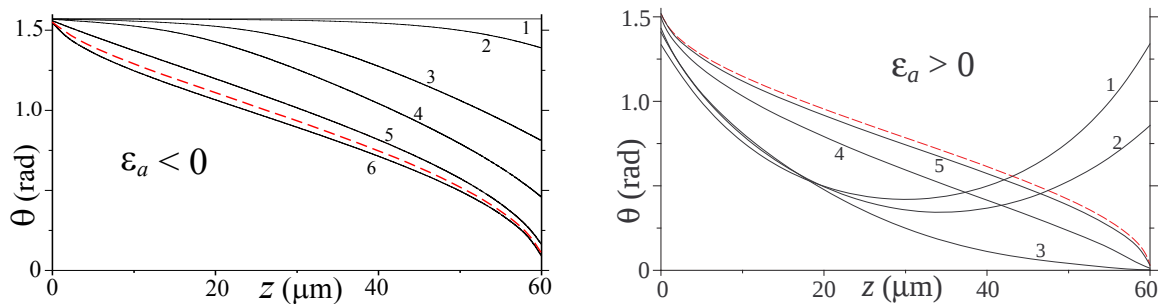


Figure 2. The profiles $\theta(z)$ for $U = 1.2 \text{ V}$. The lines in the case of $\varepsilon_a < 0$: 1 – $\bar{e} = 10^{-3}$, 2 – $\bar{e} = 1.5 \times 10^{-3}$, 3 – $\bar{e} = 1.8 \times 10^{-3}$, 4 – $\bar{e} = 2 \times 10^{-3}$, 5 – $\bar{e} = 3 \times 10^{-3}$, 6 – $\bar{e} = 10^{-2}$ in statC/cm units; lines in the case of $\varepsilon_a > 0$: 1 – $\bar{e} = 0$, 2 – $\bar{e} = 10^{-4}$, 3 – $\bar{e} = 10^{-3}$, 4 – $\bar{e} = 3 \times 10^{-3}$, 5 – $\bar{e} = 10^{-2}$ in statC/cm units. The dashed lines correspond to the dependence $\cos^2 \theta(z) \simeq z/L$.

$\varepsilon_a < 0$ and $\varepsilon_a > 0$. However, with the increase of $\bar{e}$ the orientational structures tend to be the same. This interesting feature can be explained as follows. The free energy (3) for high $\bar{e}$ and/or large U (when K_{ii} - and $W_{\theta,\varphi}^{(\alpha)}$ -terms in the free energy can be neglected) can be reduced to

$$\mathcal{F} \simeq -\frac{S_{\perp}}{8\pi}U^2J + S_{\perp}\bar{e}UJJ_1 + 2\pi S_{\perp}\bar{e}^2 \int_0^L \frac{(\sin 2\theta \theta' - JJ_1)^2}{\mathcal{E}(\theta)} dz. \quad (10)$$

Note that when the terms containing $\bar{e}$ are much greater than the first term in (10), the minimum of this functional is given by $\cos^2 \theta(z) \simeq z/L$ for the both cases, $\varepsilon_a < 0$ and $\varepsilon_a > 0$. Thus for rather high $\bar{e}$ the hybrid structure will occur. In such structure in the neighborhood of one boundary, the molecules are on the average parallel to the boundary plane, and near the other – perpendicular. The transition between the planar helicoidal and the hybrid structures may give rise to the development of new flexoelectricity-based switching devices.

The orientational transition of a new type was found in CLC with sufficiently high value of $\bar{e}$. This transition is illustrated in Fig. 3, where we present $\theta(z)$ -profiles for the fixed $\bar{e}$ and different voltages. With the increase of the external voltage from the zero value a continuous Frèedericksz transition occurs. With the further increase in voltage, another transition takes place. It is a discontinuous transition between two essentially different orientational structures. Jumps between lines 2 and 3 in Fig. 3 correspond to this new transition. Note, that for very

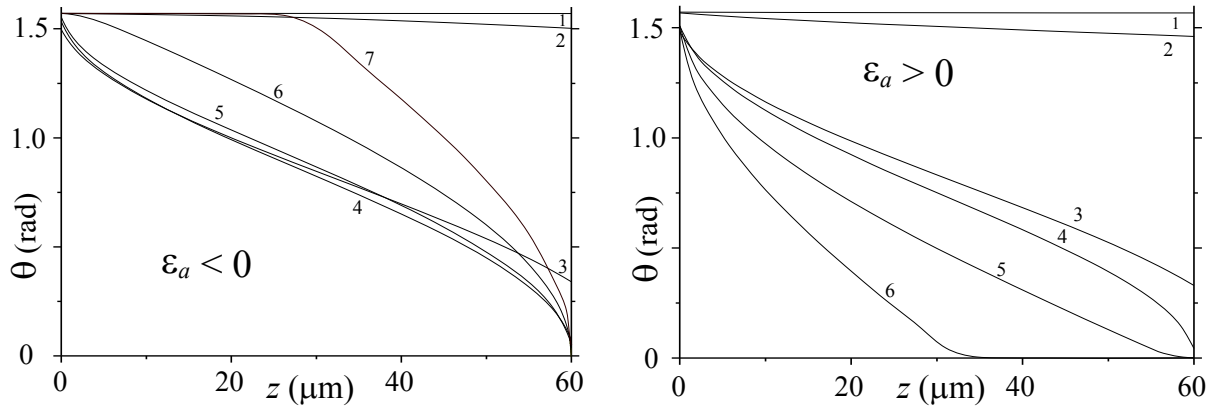


Figure 3. The equilibrium structure of $\theta(z)$ for $\bar{e} = 0.01$ statC/cm. The lines in the case of $\varepsilon_a < 0$: 1 – $U = 0.15$ V, 2 – $U = 0.17$ V, 3 – $U = 0.18$ V, 4 – $U = 1$ V, 5 – $U = 2$ V, 6 – $U = 5$ V and 7 – $U = 10$ V; lines in the case of $\varepsilon_a > 0$: 1 – $U = 0.15$ V, 2 – $U = 0.17$ V, 3 – $U = 0.18$ V, 4 – $U = 1$ V, 5 – $U = 5$ V and 6 – $U = 10$ V.

high voltage U the first term in Eq. (10) becomes dominating. Hence the system tends to the saturation structure inside the cell, which is $\theta(z) = \pi/2$ for $\varepsilon_a < 0$ and $\theta(z) = 0$ for $\varepsilon_a > 0$.

Acknowledgments

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