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FLEXOELECTRIC TORQUE IN UNIFORMLY LYING HELIX STRUCTURES OF CHIRAL NEMATIC LIQUID CRYSTALS

Electric field induced deformations of chiral nematic liquid crystal layers were studied numerically. Uniformly lying helix structure of short pitch flexoelectric mixtures was considered. The electro-optic effect due to rotation of optical axis around the normal to the layer was simulated. The flexoelectric torque arising under the action of bias voltage and responsible for this rotation was calculated. It was found that the prevailing torque occurs in close vicinity of the boundary plates. Nonlinearity of superposition of splay and bend contributions to the total flexoelectric torque was found.

Keywords: chiral nematic, helical axis, flexoelectro-optic effect.

1. INTRODUCTION

Chiral nematic liquid crystals of pitch p shorter than visible light wavelength behave as uniaxial birefringent medium with optic axis parallel to the helix axis [1]. The twisted cholesteric structure within the layer confined between plane-parallel plates is incompatible with homeotropic boundary conditions. Therefore the subsurface regions are deformed by splay and bend. If the liquid crystal possesses flexoelectric properties then the deformation is accompanied by polarization of flexoelectric nature. An interesting linear electro-optic effect is possible under the action of the electric field of strength E applied perpendicular to the layer. The field interacts with the polarization and causes director rotation around the normal to the layer by a small angle Φ [1-3]. This effect results in change of orientation of the optical axis, which in this case is perpendicular to the twisted director (Fig. 1.). Interactions of dielectric nature are undesirable, because they induce a quadratic electro-optic effect and may lead to unwinding of the helical structure. Therefore the dielectric anisotropy of the

nematic should be zero or as small as possible. The rotation angle is approximately proportional to the electric field strength, according to the simplified formula

$$\Phi(E) = \frac{eEp}{2\pi k} \quad (1)$$

where e and k are the effective flexoelectric coefficient and the effective elastic constant, respectively [3]. The direction of deviation depends on the field sign. In the most favourable case, the angle Φ reaches $\pm 22.5^\circ$ which allows to switch between transmission 0 and 1 if the layer is placed between crossed polarizers [2]. The switching times are below 1 millisecond [4,5].

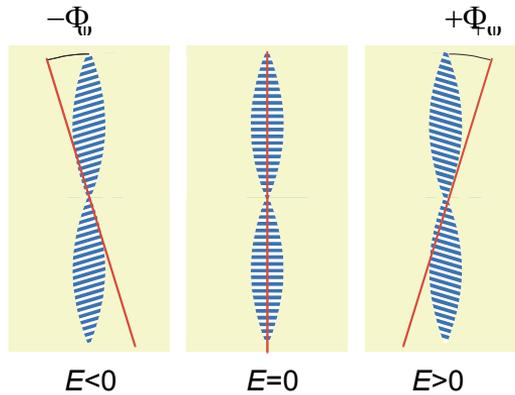


Fig. 1. Deviation of the optic axis under the action of electric field

2. ASSUMPTIONS AND METHOD

The aim of the present paper is to study the spatial distribution of flexoelectric torque responsible for rotation of the optical axis around the z axis. In particular it is interesting what is the role of flexoelectric coefficients e_{11} and e_{33} connected with splay and bend, respectively. For this purpose, the chiral nematic liquid crystal layer of thickness $d = 2 \mu\text{m}$ was taken into account. The layer was parallel to the xy plane of the coordinate system. It was placed between two electrodes positioned at $z = \pm d/2$. The helical axis was directed along the y axis. Director orientation was determined by the polar angle $\theta(y,z)$ made between the director and its projection on the xy plane, and by the azimuthal angle $\phi(z)$ between this projection and the x axis. Both angles as well as all other quantities were independent of the x coordinate. The azimuthal angle was assumed to be independent of y . The chirality of the nematic was determined by the intrinsic pitch, smaller than wavelength of visible light,

$p = 0.3 \mu\text{m}$. Homeotropic boundary conditions were assumed. The anchoring energy was determined by the polar and azimuthal anchoring strength coefficients, $W_\theta = 10^{-4}$ and $W_\phi = 10^{-5} \text{Jm}^{-2}$, respectively ([6]). Dielectric anisotropy was assumed to be zero. Three sets of the flexoelectric coefficients were considered:

1. $e_{11} = 10 \text{ pC/m}$, $e_{33} = 0$,
2. $e_{11} = 0$, $e_{33} = -10 \text{ pC/m}$,
3. $e_{11} = 10 \text{ pC/m}$, $e_{33} = -10 \text{ pC/m}$.

Typical elastic constants were adopted: $k_{11} = 8 \text{ pN}$, $k_{22} = 4 \text{ pN}$, $k_{33} = 12 \text{ pN}$. The layer was subjected to voltage U ranging from 0 to 10 V. Nematic of high purity was assumed i.e. the presence of ions was neglected.

The deformation of the layer is caused by torque of flexoelectric origin (since $\Delta\varepsilon$ is assumed to be zero) which is given by vector product $\mathbf{\Gamma} = \mathbf{P} \times \mathbf{E}$, where $\mathbf{P} = e_{11}(\mathbf{n} \cdot \nabla \mathbf{n}) - e_{33}(\mathbf{n} \times (\nabla \times \mathbf{n}))$ and $\mathbf{E} = -\nabla V$. In order to find the z -component of the torque responsible for rotation of the optical axis, $\Gamma_z = P_x E_y$, the director distribution over the cross section of the layer segment of width p was calculated. The minimization energy method described in detail in earlier papers was used for this purpose. The electric potential distribution $V(y, z)$ was also determined by resolving of the Poisson equation [7]. The calculations yielded the x -component of the flexoelectric polarization

$$P_x = e_{11} n_x \left(\frac{\partial n_y}{\partial y} + \frac{\partial n_z}{\partial z} \right) + e_{33} \left(n_y \frac{\partial n_x}{\partial y} + n_z \frac{\partial n_x}{\partial z} \right) \quad (2)$$

as well as the y -component of electric field strength

$$E_y = -\frac{\partial V}{\partial y} \quad (3)$$

which allowed to determine Γ_z .

3. RESULTS AND DISCUSSION

The typical deformation of the helical structure is presented in Fig. 2 by means of cylinders symbolizing the director. The azimuthal angle which measured the director rotation around the normal to the layer was found to adopt the same value in the prevailing part of the cross section with exception of thin subsurface regions. This value was taken as the rotation angle of the optic axis Φ . The director distribution is analogous to the pattern presented by Bouligand [3,8] i.e. it is composed of regions of splay and bend deformations. The spatial period of the deformed structure is equal to $p/2$ just like in the undisturbed chiral nematics in which the properties are repeated every half of pitch due to identity

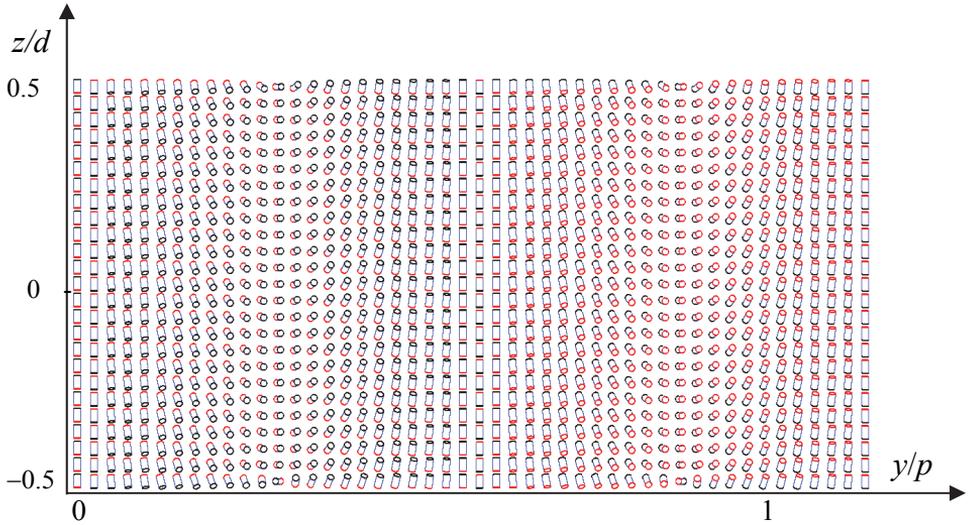


Fig. 2. Director distribution in the cross section of the layer along the pitch; $p = 0.3 \mu\text{m}$, $e_{11} = 10 \text{ pC/m}$, $e_{33} = -10 \text{ pC/m}$, $U = 12 \text{ V}$.

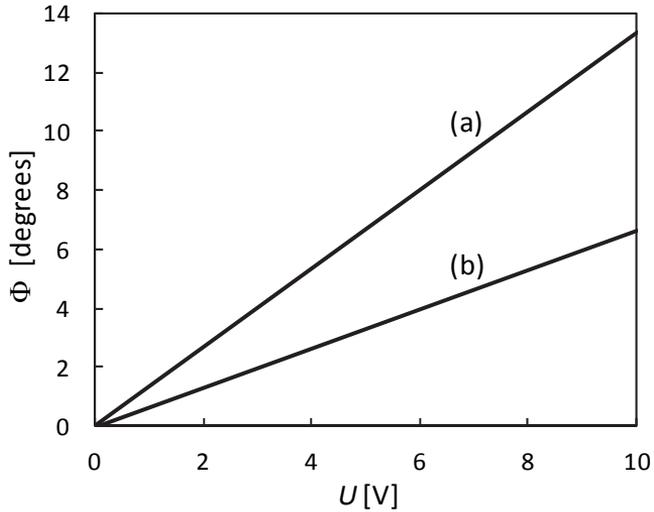


Fig. 3. Deviation angle Φ as a function of bias voltage; curve (a): $e_{11} = 10 \text{ pC/m}$ and $e_{33} = -10 \text{ pC/m}$; curve (b): $e_{11} = 10 \text{ pC/m}$ and $e_{33} = 0$ as well as $e_{11} = 0$ and $e_{33} = -10 \text{ pC/m}$; (both sets of flexoelectric coefficients give identical results).

$\mathbf{n} \equiv -\mathbf{n}$. The field induced deformations realized with the three mentioned sets of flexoelectric coefficients are qualitatively the same. In Fig. 3, the voltage dependencies of the angle Φ calculated for the three sets of flexoelectric coefficients are compared. It is evident that separate contributions of $e_{11} = 10$ pC/m and $e_{33} = -10$ pC/m to the electro-optic effect are identical due to equality $e_{11} = -e_{33}$ (curve b), whereas the simultaneous contributions of both coefficients lead to doubled rotation angles (curve a). It was also checked that rotation does not occur if $e_{11} = e_{33}$ i.e. if $e_{11} - e_{33}$ vanishes. The above statements are coherent with theoretical predictions that the angle Φ depends on difference of flexocoefficients, $e_{11} - e_{33}$, and not on their particular values [2].

The exemplary flexoelectric torques responsible for rotation of optical axis are illustrated in Figs. 4-6 as functions of y and z . The distributions are symmetrical with respect to $y = p/2$ i.e. $\Gamma_z(y) = \Gamma_z(p - y)$. This means that the spatial period of the torque is equal to p in contrary to the spatial period $p/2$ of the director distribution. Such property is due to the symmetries of the polarization and electric field components expressed by relations $P_x(y) = -P_x(p - y)$ and $E_x(y) = -E_x(p - y)$, respectively.

The flexoelectric torque counteracts the subsurface anchoring torque and the elastic torque in the bulk. It reaches the highest values at the boundary plates and in the regions where the director components n_x , n_y and n_z as well as their spatial derivatives have significant values. The equilibrium between the flexoelectric, elastic and anchoring torques can be achieved at high as well as at low values of flexoelectric torque and it can result in non-zero rotation angle Φ . Comparison of Figs. 4-6 with Fig. 2 shows that no torque is induced in the vicinity of $y/p = 0.25$ and $y/p = 0.75$. This is due to the fact that the deformation contains neither splay nor bend in those regions, therefore the flexoelectric polarization is zero. In the region surrounding $y/p = 0.5$, the n_x and n_y components are practically zero and the n_z component weakly depends on z therefore P_x (Eq. (2)) is negligible. The torque vanishes also at $y/p = 0$ and $y/p = 1$ for similar reasons.

The spatial distributions of torque over the cross section of the layer are rather complicated. The torque distributions vary with voltage. They arise as a result of self consistency between director field deformations producing flexoelectric polarization and interactions of the polarization with external electric field which also influence the director orientation.

In the case of $e_{11} = 10$ pC/m, $e_{33} = -10$ pC/m, (Fig. 4), both splay and bend give rise to the flexoelectric polarization and to the torque. The largest Γ_z values occur in the subsurface regions, in particular at $z = d/2$ and correspond to significant variations of director orientation. The small opposite torque occurs at

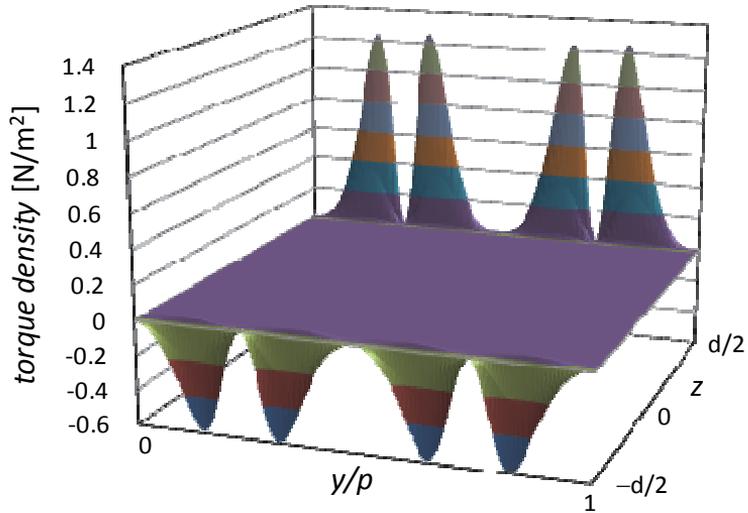


Fig. 4. Torque per unit volume as a function of position in the cross section of the layer; $p = 0.3 \mu\text{m}$, $e_{11} = 10 \text{ pC/m}$, $e_{33} = -10 \text{ pC/m}$, $U = 8 \text{ V}$.

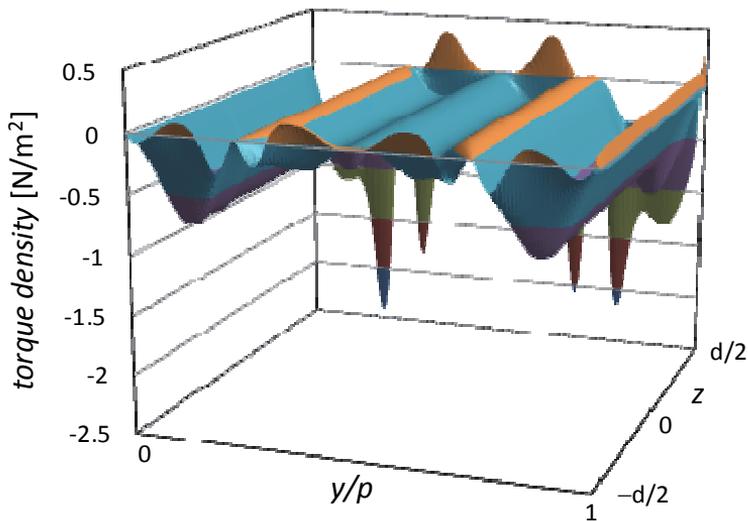


Fig. 5. Torque per unit volume as a function of position in the cross section of the layer; $p = 0.3 \mu\text{m}$, $e_{11} = 0 \text{ pC/m}$, $e_{33} = -10 \text{ pC/m}$, $U = 8 \text{ V}$.

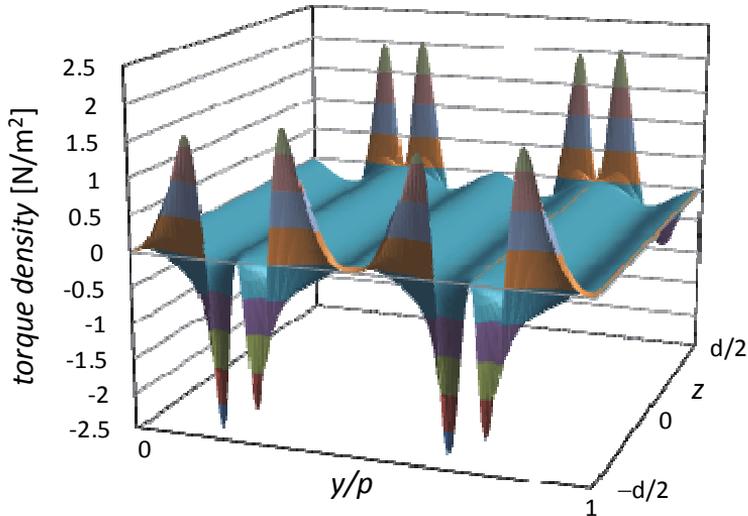


Fig. 6. Torque per unit volume as a function of position in the cross section of the layer; $p = 0.3 \mu\text{m}$, $e_{11} = 10 \text{ pC/m}$, $e_{33} = 0 \text{ pC/m}$, $U = 8 \text{ V}$.

$z = -d/2$ whereas the torques in prevailing part of the cross section are practically inessential. Much more complex distributions occur in the two other situations shown in Figs. 5 and 6. Significant torques arise not only in the vicinity of the boundary plates but also in the bulk of the layer. In particular, four regions of non-zero torques can be distinguished along the pitch. It is also evident that sum of the torque distributions occurring when either e_{11} or e_{33} are zero does not give the distribution arising when both flexoelectric coefficients do not vanish. This is an example of nonlinear superposition which is the pronounced manifestation of complexity of elastic, flexoelectric and surface interactions leading to equilibrium structures.

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FLEXOELEKTRYCZNY MOMENT SIŁ W STRUKTURACH NEMATYKÓW CHIRALNYCH Z OSIĄ HELISY LEŻĄCĄ W PŁASZCZYŹNIE WARSTWY

Streszczenie

Zbadano numerycznie odkształcenia warstw nematyków chiralnych wywołane polem elektrycznym. Obliczenia dotyczyły nematyka o krótkim okresie struktury i właściwościach fleksoelektrycznych z osią helisy równoległą do płaszczyzny warstwy. Symulowano efekt elektrooptyczny polegający na obrocie osi optycznej warstwy wokół normalnej do płaszczyzny warstwy. Obliczono fleksoelektryczny moment sił powstający pod wpływem zewnętrznego napięcia i odpowiedzialny za ten obrót. Pokazano, że przeważający moment sił powstaje w pobliżu elektrod. Stwierdzono nieliniowy charakter superpozycji rozkładów momentów polegający na tym, że suma rozkładów momentów istniejących gdy $e_{11} = 0$ lub $e_{33} = 0$ różni się od rozkładu powstającego gdy oba współczynniki są różne od zera.