Deformations of nematic layers induced by electric field were studied numerically. The role of very strong flexoelectric properties was considered. The threshold voltages for deformations were calculated for nematics with very low, moderate and high ion contents and characterized by negative dielectric anisotropy. The director distributions were also determined. When the sum of flexoelectric coefficients reached large values, the threshold voltage significantly decreased. The strong flexoelectric properties caused that even for extremely pure materials the threshold was lower than the theoretical value calculated for perfectly insulating material.

Keywords: flexoelectricity, nematic layers, electric field induced deformations.

1. INTRODUCTION

Deformations of nematic liquid crystal layers induced by external electric field are due to torques acting on director which may have dielectric and flexoelectric nature. When the electric field is applied perpendicular to the layer plane, the deformations arise above some threshold voltage. The threshold value depends on dielectric anisotropy $\Delta \varepsilon$, sum of the flexoelectric coefficients $e = e_{11} + e_{33}$, anchoring energy $W$, ion mobilities $\mu^+$ and ion concentrations $N^\pm$. In previous papers, some of these relationships were investigated [1-5]. In this paper, the role of strong flexoelectric properties in the electric field induced deformations is studied numerically.

A homeotropic layers containing flexoelectric nematic liquid crystal was taken into account. The threshold voltage for deformations were calculated for
nematic materials of various purity level, characterized by very low, moderate and high ion content. The director distributions in the deformed states were also determined.

The main results are as follows: (i) the strong flexoelectric properties lead to drastic decrease of the threshold voltage; (ii) even for extremely pure materials containing as low ion concentration as $10^{17} \text{m}^{-3}$, the threshold is lower than the theoretical value calculated for perfectly insulating material; (iii) the influence of flexoelectricity on the behaviour of the nematic layer strongly depends on the ion content; (iv) in the case of high ion concentration and strong flexoelectric properties, the form of director distributions is qualitatively the same for various values of $e$.

2. GEOMETRY AND PARAMETERS

A nematic liquid crystal layer of thickness $d = 20 \mu \text{m}$ was confined between two infinite plates parallel to the $xy$ plane of the Cartesian co-ordinate system. They were positioned at $z = \pm d/2$ and played the role of electrodes. The voltage $U$ was applied between them; the lower electrode ($z = -d/2$) was earthed. Homeotropic alignment, identical on both boundary plates, was assumed. The anchoring strength $W$ was $10^{-5} \text{Jm}^{-2}$. The director orientation was described by the angle $\theta(z)$, measured between the director $\mathbf{n}$ and the $z$ axis. The model substance was characterized by the elastic constants $k_{11} = 6.2 \times 10^{-12} \text{N}$ and $k_{33} = 8.6 \times 10^{-12} \text{N}$. The dielectric anisotropy, $\Delta \varepsilon = -0.7$, were taken into account (dielectric constant components were equal to $\varepsilon_\parallel = 4.7$ and $\varepsilon_\perp = 5.4$). The flexoelectric properties were expressed by the sum of the flexoelectric coefficients $e_{11} + e_{33}$, which ranged from 40 to 200 pCm$^{-1}$ (the separate values of $e_{11}$ and $e_{33}$ are not essential in the considered geometry [6]).

The weak electrolyte model was adopted for the description of electrical phenomena in the layer [7]. The ion concentrations were determined by the generation constant and recombination constant. The transport of ions in the layer was described by typical values of mobility coefficients and diffusion coefficients. It was assumed that the mobility of anions was larger than that of cations: $\mu^-_i = 1.5 \times 10^{-9}$, $\mu^-_c = 1 \times 10^{-9}$, $\mu^+_i = 1.5 \times 10^{-10}$, $\mu^+_c = 1 \times 10^{-10} \text{m}^2\text{V}^{-1}\text{s}^{-1}$, i.e. $\mu^+_i / \mu^+_c = 1.5$. The Einstein relation was assumed for the diffusion constants: $D_{\parallel \perp} = (k_B T / q ) \mu_{\parallel \perp}^\pm$, where $q$ denotes the absolute value of the ionic charge, $k_B$ is Boltzmann constant and $T$ – absolute temperature. The $z$-components of mobilities and of diffusion coefficients are given by $\mu_{\pm z}^\pm = \mu_{\pm}^\pm + \Delta \mu^\pm \cos^2 \theta$ and
Deformations of nematics with strong flexoelectric properties

\[ D^z = D_0^z + \Delta D^z \cos^2 \theta, \text{ where } \Delta \mu^z = \mu^z_i - \mu^z_{\perp} \text{ and } \Delta D^z = D_0^z - D_{\perp}^z. \]

The generation constant \( \beta \) depended on the electric field strength \( E \): \( \beta = \beta_0 \left[ 1 + \frac{|E|^3}{8\pi \varepsilon \varepsilon_0 k_B T^2} \right] \), [8], where \( \varepsilon = (\varepsilon_\perp + \varepsilon_i) / 3 \) and \( \beta_0 \) was varied from \( 10^{18} \) to \( 10^{24} \) m\(^{-2}\)s\(^{-1}\). The recombination constant \( \alpha = 2q\mu / (\varepsilon_0 \varepsilon) \), [8], where \( \mu = \left[ (2\mu_i^+ + \mu_i^+) / 3 + (2\mu_i^- + \mu_i^-) / 2 \right] / 2 \), was equal to \( 4.5 \times 10^{-18} \) m\(^3\)s\(^{-1}\).

In thermodynamic equilibrium, the ion concentration \( N_0 = \sqrt{\beta_0 / \alpha} \) was of the order \( 10^{17} \div 10^{21} \) m\(^{-3}\) and represented the low, moderate and high ion content.

3. METHOD

The problem was considered to be one-dimensional. The functions \( \theta(z) \), \( V(z) \) and \( N^0(z) \), which describe the director orientation, the potential and ion concentration distribution within the layer, respectively, were calculated by resolving of the set of ten equations which consisted of equation of balance of elastic, dielectric and flexoelectric torques for the bulk, two equations of balance of elastic, flexoelectric and anchoring torques for the boundaries, the Poisson equation, two continuity equations for the ion fluxes, four equations for ion concentrations on the boundaries [1]. This allowed to determine the threshold voltages for the deformations and the director field in the deformed layers.

The transport of ions in the bulk and across the electrode-nematic interfaces was described in terms of a model presented in details in the earlier papers [1,9]. The conducting properties of the layer were characterized by the rate of the neutralization of ions as well as the rate of their generation. The rates of the both electrode processes were determined by a single parameter \( K_r \). Its value, \( K_r = 10^{-7} \) ms\(^{-1}\), represented the quasi-blocking character of the electrode contacts, i.e. it reflected the high resistance of the contact.

4. RESULTS

4.1. Threshold voltage

The threshold voltages for deformations were calculated for various values of the sum of flexoelectric coefficients \( e_{11} + e_{33} \) and for six ion concentrations \( N_0 \). The results are shown in Figures 1 and 2. The calculated threshold voltages
are lower than the theoretical values corresponding to the insulating nematic even in the case of the lowest ion content, \( N_0 = 5 \times 10^{17} \text{ m}^{-3} \). They decrease with increasing ion concentrations as well as with increasing flexoelectric properties. For every ion content, the strong flexoelectric properties lead to drastic decrease of the threshold voltage down to values below 0.1 V.

![Fig. 1. Threshold voltages as a function of the sum of flexoelectric coefficients.](image1)

The ion concentrations \( N_0 \) in \( \text{m}^{-3} \) are indicated at the curves

![Fig. 2. Threshold voltages as a function of the ion concentrations.](image2)

The values of \( \epsilon_{11} + \epsilon_{33} \) in \( \text{pC m}^{-1} \) are indicated at the curves
4.2. Director distributions

In order to determine qualitative character of the deformations arising for strong values of flexoelectric coefficients, the director distribution were calculated for voltages exceeding the thresholds by 0.1 V. They are exemplified in Figures 3-5. Their form can be interpreted by means of torques which are determined by the electric field distributions.

For very low ion content and relatively weak flexoelectric properties, the deformations are nearly symmetrical. The director distributions resemble the deformations predicted theoretically for the insulating nematics \((e_{11} + e_3 = 40 \text{ pCm}^{-1})\). For increasing flexoelectric coefficients, asymmetry of director distribution appears. This is due to bulk flexoelectric torque acting in the left half of the layer caused by electric field gradient in this region. Similar but more pronounced effect is observed for higher ion concentration, as presented in Figure 4.

For the highest ion concentrations, \(N_0 = 10^{20} \text{ m}^{-3}\), the deformations are stronger. They increase with flexoelectric coefficients and have a different character (Fig. 5). Their form is mainly due to the action of large subsurface electric field gradients and to very strong surface fields induced by the space charge of separated ions. This field distribution leads to bulk flexoelectric torques destabilizing in the vicinity of the cathode and stabilizing in
Fig. 4. The director distributions for moderate ion concentration $N_0 = 10^{18} \text{ m}^{-3}$. The values of $e_{11} + e_{33}$ in pCm$^{-1}$ are indicated at the curves.

Fig. 5. The director distributions for high ion concentration $N_0 = 10^{20} \text{ m}^{-3}$. The values of $e_{11} + e_{33}$ in pCm$^{-1}$ are indicated at the curves.
Deformations of nematics with strong flexoelectric properties

the neighbourhood of the anode and to surface torques which are stabilizing at
the cathode and destabilizing at the anode. As a result, the angle describing the
director orientation in the prevailing part of the layer varies almost linearly with
the $z$ co-ordinate. The effect of the dielectric torque is negligible.

5. SUMMARY AND DISCUSSION

In the present paper, the strong flexoelectric properties were assumed which
is supported by the results reported in [10] for the bent-core nematic mesogen.
However some newer measurements showed that the flexoelectric coefficients
for the same material have rather typical values of the order $10\pm10^2$ pCm$^{-1}$ [11].
Nevertheless, the role of enhanced flexoelectric coefficients for the deformations
of nematic layers is worthy to be studied.

The results presented in this paper show that the influence of
flexoelectricity on the behaviour of the nematic layer is strongly related to the
presence of ions. This concerns both the threshold voltage as well as the director
distributions. When the sum of flexoelectric coefficients reaches large values,
the threshold voltage decreases strongly. The strong flexoelectric properties
cause that even for extremely pure materials the threshold is lower than the
theoretical value calculated for perfectly insulating material. In the case of large
values of $e_{11} + e_{33}$ and for $N_0 > 10^{18}$ m$^{-3}$, the director distributions adopt the form
determined by the flexoelectric torques induced by surface electric fields and
subsurface field gradients. This form is qualitatively the same for various values
of $e$ and weakly depends on the ion concentration. However the magnitude of
deformations is strongly influenced by the ion content. This indicates that in the
case of strong flexoelectric properties, the ion concentration should be as low as
possible and thoroughly controlled.

REFERENCES

Streszczenie