SCIENTIFIC BULLETIN OF THE TECHNICAL UNIVERSITY OF LODZ
No. 1082 Physics, Vol. 31 2010

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INFLUENCE OF STRONG FLEXOELECTRIC PROPERTIES ON DEFORMATIONS OF NEMATIC LIQUID LAYERS INDUCED BY DC ELECTRIC FIELD

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 $\mu^{\pm}$ 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} 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 $d = 20$ µm 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} Jm^{-2}. The director orientation was described by the angle $\theta(z)$, measured between the director **n** and the z axis. The model substance was characterized by the elastic constants $k_{11} = 6.2\cdot10^{-12}$ N and $k_{33} = 8.6\cdot10^{-12}$ 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: $\mu_{\parallel}^{-} = 1.5\cdot10^{-9}$, $\mu_{\perp}^{-} = 1\cdot10^{-9}$, $\mu_{\parallel}^{+} = 1.5\cdot10^{-10}$, $\mu_{\perp}^{+} = 1\cdot10^{-10}$ m^{2}V^{-1}s^{-1}, i.e. $\mu_{\parallel}^{\pm}/\mu_{\perp}^{\pm} = 1.5$. The Einstein relation was assumed for the diffusion constants: $D_{\parallel,\perp}^{\pm} = (k_B T/q)\,\mu_{\parallel,\perp}^{\pm}$ 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 $\mu_{zz}^{\pm} = \mu_{\perp}^{\pm} + \Delta\mu^{\pm}\cos^2\theta$ and

$D_{zz}^{\pm} = D_{\perp}^{\pm} + \Delta D^{\pm}\cos^2\theta$, where $\Delta\mu^{\pm} = \mu_{\parallel}^{\pm} - \mu_{\perp}^{\pm}$ and $\Delta D^{\pm} = D_{\parallel}^{\pm} - D_{\perp}^{\pm}$. The generation constant β depended on the electric field strength E: $\beta = \beta_0\left[1 + |E|q^3/\left(8\pi\varepsilon\,\varepsilon\,k_B^2T^2\right)\right]$, [8], where $\varepsilon = \left(2\varepsilon_{\perp} + \varepsilon_{\parallel}\right)/3$ and β_0 was varied from 10^{18} to 10^{24} $\mathrm{m^{-3}s^{-1}}$. The recombination constant $\alpha = 2q\mu/\left(\varepsilon_0\varepsilon\right)$, [8], where $\mu = \left[\left(2\mu_{\perp}^{+} + \mu_{\parallel}^{+}\right)/3 + \left(2\mu_{\perp}^{-} + \mu_{\parallel}^{-}\right)/3\right]/2$, was equal to 4.5×10^{-18} $\mathrm{m^3s^{-1}}$. In thermodynamic equilibrium, the ion concentration $N_0 = \sqrt{\beta_0/\alpha}$ was of the order $10^{17} \div 10^{21}$ $\mathrm{m^{-3}}$ 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 $N^{\pm}(z)$, 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, $K_r = 10^{-7}$ $\mathrm{ms^{-1}}$, 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, $N_0 = 5{\cdot}10^{17}$ 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.

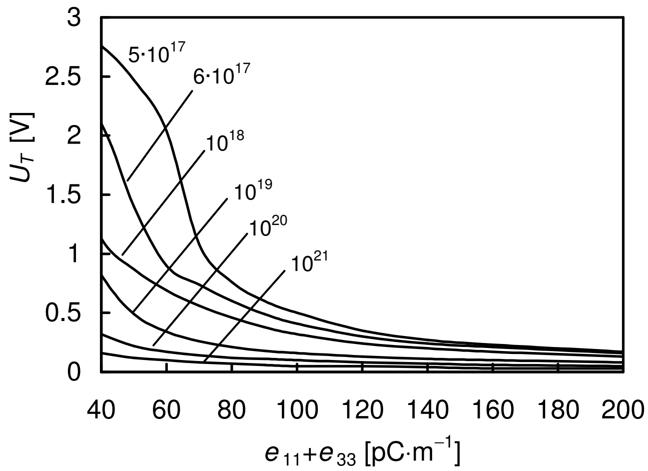

Fig. 1. Threshold voltages as a function of the sum of flexoelectric coefficients. The ion concentrations N_0 in m^{-3} are indicated at the curves

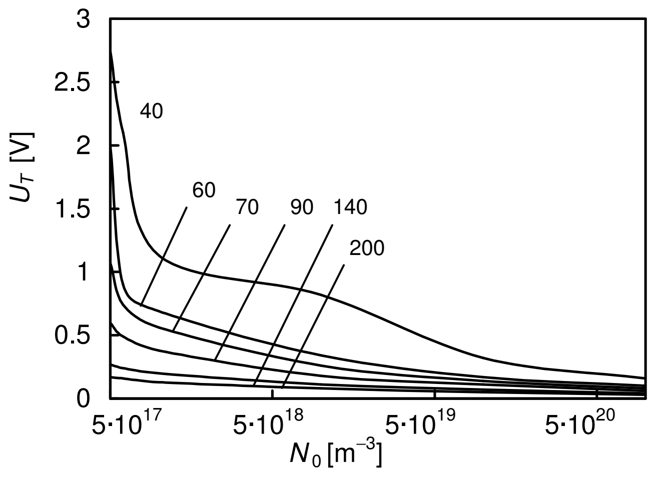

Fig. 2. Threshold voltages as a function of the ion concentrations. The values of $e_{11}+e_{33}$ in pCm^{-1} are indicated at the curves

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.

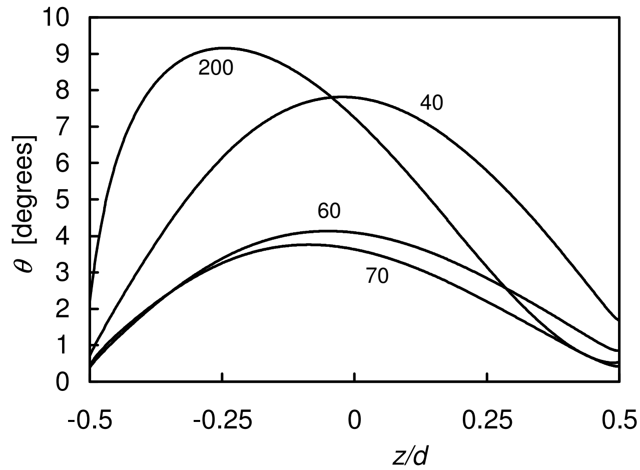

Fig. 3. The director distributions for very low ion concentration $N_0 = 5 \cdot 10^{17}$ m^{-3}. The values of $e_{11}+e_{33}$ in pCm^{-1} are indicated at the curves

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 ($e_{11}+e_3 = 40$ 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, $N_0 = 10^{20}$ 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

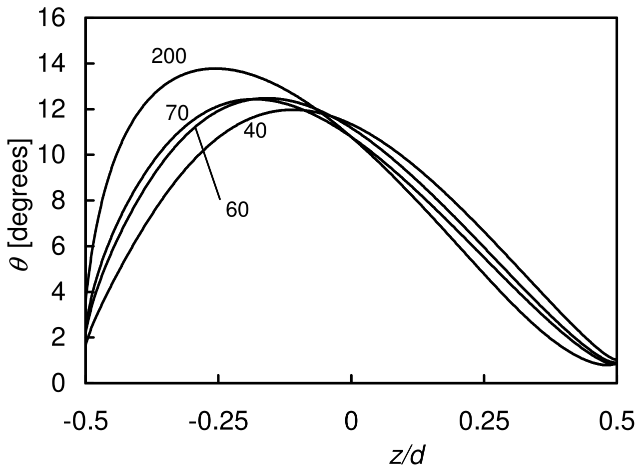

Fig. 4. The director distributions for moderate ion concentration $N_0 = 10^{18}$ m^{-3}. The values of e_{11}+e_{33} in pCm^{-1} are indicated at the curves

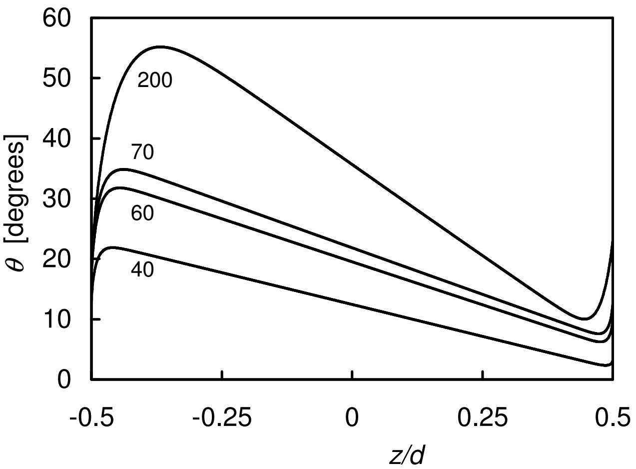

Fig. 5. The director distributions for high ion concentration $N_0 = 10^{20}$ m^{-3}. The values of e_{11}+e_{33} in pCm^{-1} are indicated at the curves

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 $10 \div 10^2$ 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

[1] **Derfel G.**, **Buczkowska M.,** Liq. Cryst., **32** (2005) 1183.
[2] **Buczkowska M.**, **Derfel G.,** Liq. Cryst., **32** (2005) 1285.
[3] **Derfel G.**, **Buczkowska M.,** Liq. Cryst., **34** (2007) 113.
[4] **Buczkowska M.**, **Derfel G.,** Sci. Bull. Tech. Univ. Lodz, No. 1030, Physics, **29** (2008) 5.
[5] **Buczkowska M.**, **Grzelczak K.,** Sci. Bull. Tech. Univ. Lodz, No. 1057, Physics, **30** (2009) 5.
[6] **Derzhanski A.**, **Petrov A.G.**, **Mitov M.D.,** J. Phys. (Paris), **39** (1978) 273.

[7] **Briere G.**, **Gaspard F.**, **Herino R.,** J. Chim. Phys. **68** (1971) 845.

[8] **de Vleeschouwer H.**, **Verschueren A., Bougriona F.**, **Van Asselt R.**, **Alexander E., Vermael S.**, **Neyts K.**, **Pauwels H.,** Jpn. J. Appl. Phys., **40** (2001) 3272.

[9] **Derfel G.,** J. Mol. Liq., **144** (2009) 59.

[10] **Harden J., Mbanga B., Eber N., Fodor-Csorba K., Sprunt S., Gleeson J.T., Jakli A.,** Phys. Rev. Lett. **97** (2006) 157802.

[11] **Khoa Van Le**, **Araoka F.**, **Fodor-Csorba K.**, **Ishikawa K.**, **Takezoe H.,** Liq. Cryst., **36** (2009) 1119.

WPŁYW SILNYCH WŁAŚCIWOŚCI FLEKSOELEKTRYCZNYCH NA DEFORMACJE WARSTW NEMATYKA WYWOŁANE STAŁYM POLEM ELEKTRYCZNYM

Streszczenie

Zbadano numerycznie odkształcenia warstw nematycznych wywołane polem elektrycznym. Rozpatrzono wpływ bardzo silnych właściwości fleksoelektrycznych. Obliczono napięcia progowe na odkształcenie dla nematyków z ujemną anizotropią dielektryczną. Wzięto pod uwagę niską, średnią i wysoką koncentrację jonów. Określono także rozkłady direktora w warstwie. W przypadku dużej sumy współczynników fleksoelektrycznych napięcie progowe znacznie się obniżało. Silne właściwości fleksoelektryczne powodowały, że nawet dla bardzo czystych materiałów napięcie progowe było znacznie niższe niż teoretyczna wartość obliczona dla materiału doskonale izolującego.