SCIENTIFIC BULLETIN OF THE TECHNICAL UNIVERSITY OF LODZ
No. 1105 Physics, Vol. 32 2011

GRZEGORZ DERFEL, MARIOLA BUCZKOWSKA
BARTŁOMIEJ PIETRZYK

Institute of Physics, Technical University of Łódź, ul. Wólczańska 219
90-924 Łódź, Poland, e-mail: gderfel@p.lodz.pl

DIRECT CURRENT ELECTRIC FIELD INDUCED DEFORMATIONS OF DIELECTRICALLY ISOTROPIC FLEXOELECTRIC NEMATIC LAYERS

Deformations of nematic layers induced by d.c. electric field were studied numerically. The nematic liquid crystal under consideration possessed flexoelectric properties. Its dielectric anisotropy was zero, so the deformations were solely of flexoelectric nature. The threshold voltages for deformations were calculated for nematics with very low, moderate and high ion content. In the case of weak flexoelectric properties, the predicted threshold voltage reached c. 100V in pure material. It decreased strongly with increasing ion content and reached values much lower than the theoretical values calculated for the perfectly insulating material. The director distributions in deformed states were also determined. Four kinds of director profiles were distinguished.

Keywords: flexoelectricity, nematic, 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 studied numerically [1-8]. In this paper, the purely flexoelectric deformations induced by the d.c. electric field in nematics with compensated dielectric anisotropy $\Delta\varepsilon = 0$ are studied numerically. Such dielectrically isotropic materials can be obtained as a mixture of two nematics – one possessing the positive dielectric anisotropy and the other characterized by the negative dielectric anisotropy [9].

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) in the case of weak flexoelectric properties, the predicted threshold voltage reached c. 100V in pure material; (ii) the threshold decreased strongly with increasing ion content, and decreasing anchoring strength and reached values much lower than the theoretical values calculated for perfectly insulating material; (iii) four kinds of director profiles were distinguished.

2. GEOMETRY AND PARAMETERS

A nematic liquid crystal layer of thickness $d = 20\,\mu\mathrm{m}$ was confined between two infinite plates parallel to the xy plane of the Cartesian coordinate system. They were positioned at $z = \pm d/2$ and acted as 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 $2\cdot10^{-5}$ Jm^{-2}. The director **n** was parallel to the xz plane and its orientation was described by the angle $\theta(z)$, measured between **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 constant components were identical: $\varepsilon_{\parallel} = \varepsilon_{\perp} = 5.4$. The flexoelectric properties were expressed by the sum of the flexoelectric coefficients $e = e_{11} + e_{33} = \pm 40\mathrm{pC/m}$ (the individual values of e_{11} and e_{33} are not essential within the considered geometry [10]).

The weak electrolyte model was adopted for the description of electrical phenomena in the layer. 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}. 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 the 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 $D_{zz}^{\pm} = D_{\perp}^{\pm} + \Delta D^{\pm}\cos^2\theta$, respectively, where $\Delta\mu^{\pm} = \mu_{\parallel}^{\pm} - \mu_{\perp}^{\pm}$ and $\Delta D^{\pm} = D_{\parallel}^{\pm} - D_{\perp}^{\pm}$ denote the anisotropies of each quantity. The generation constant β depended on the electric field strength E: $\beta = \beta_0\left(1 + \frac{|E|q^3}{8\pi\varepsilon\,\varepsilon\, k_B^2 T^2}\right)$, where $\bar{\varepsilon} = \varepsilon_{\perp} = \varepsilon_{\parallel}$ and β_0 was varied from 10^{18} to 10^{24} m^{-3}s^{-1}. The recombination constant $\alpha = 4.32\cdot10^{-18}$ m^{3}s^{-1} was calculated from the formula $\alpha = \frac{2q\bar{\mu}}{\varepsilon_0\varepsilon}$, where $\bar{\mu} = \left[\left(2\mu_{\perp}^{+} + \mu_{\parallel}^{+}\right)/3 + \left(2\mu_{\perp}^{-} + \mu_{\parallel}^{-}\right)/3\right]/2$, [11]. In the thermodynamic equilibrium, the ion concentration N_0 was equal to $\sqrt{\beta_0/\alpha}$. The resulting ion concentrations N_0 represented the low, moderate and high values of ion content and covered the range $3\cdot10^{17} \div 3\cdot10^{20}$ m^{-3}.

3. METHOD

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

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, 12]. 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 as a function of the ion concentration N_0 for both signs of the sum of flexoelectric coefficients $e = e_{11} + e_{33}$. The results are shown in fig. 1. In the case of weak flexoelectric properties and for very low ion concentrations, the threshold voltages have rather large values reaching 100 V. Such values are much above the threshold for electrohydrodynamic effects which obviously are not taken into account by our static model. Therefore, we present our results restricted to voltages smaller than the arbitrarily chosen value of 12 V.

In general, the threshold voltages decrease when the flexoelectric properties expressed by $|e|$ become stronger. In the case of the lowest ion content, $N_0 = 3{\cdot}10^{17}$ m^{-3}, the calculated threshold coincides with the theoretical value corresponding to the insulating nematic. For the negative e value, the threshold voltages decrease monotonically with increasing ion concentrations. When the flexoelectric parameter e is positive, then there exist a narrow range of moderate ion concentrations in vicinity of $N_0 = 10^{18}$ m^{-3}, at which the deformations arise in two ranges of voltage. They appear at the low threshold, decay at some higher voltage and reappear at the high threshold. This effect was observed in our earlier studies [3,4,8]. It is due to the interaction of the flexoelectric polarisation with the gradient of electric field which has asymmetrical distribution caused by the difference between the mobilities of anions and cations. When the ion content exceeds c. $N_0 = 10^{20}$ m^{-3}, the threshold is much smaller than the theoretical value predicted for insulating material. For $|e| > 40$ pC/m it reaches extremely low values of several tenth of volt.

4.2. Director distributions

In order to determine qualitative character of the deformations of purely flexoelectric nature, the director distributions were calculated for voltages exceeding the thresholds by 10%. Figure 2 presents the four kinds of director profiles $\theta(\zeta)$ (where $\zeta = z/d$ is a reduced coordinate) arising in nematics with low ($3{\cdot}10^{17}$ m^{-3}), moderate (10^{18} and $3{\cdot}10^{18}$ m^{-3}) and high ion concentration (10^{20} m^{-3}). Their form can be interpreted by means of flexoelectric torques which are determined by the electric field distributions.

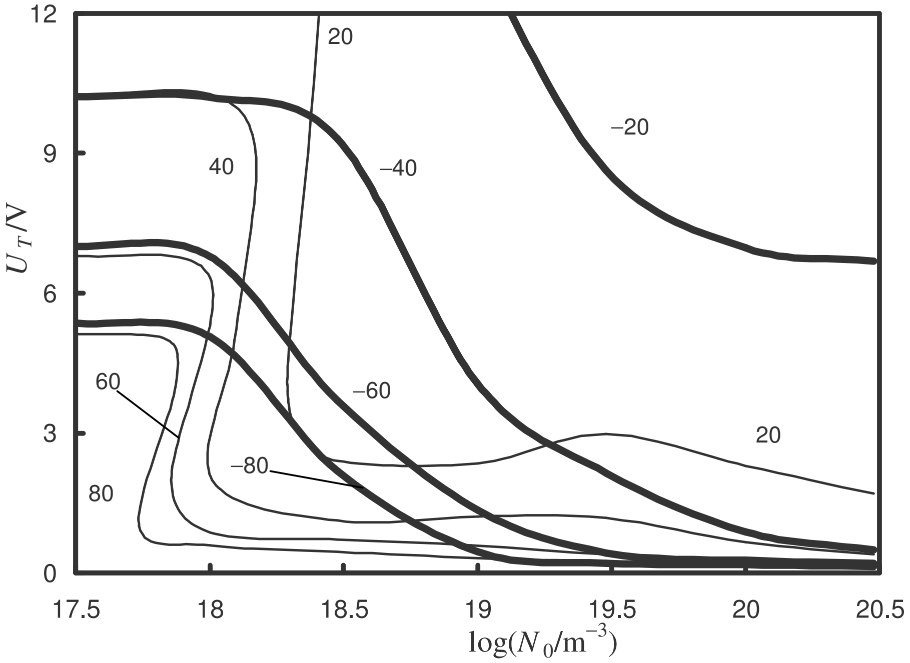

Fig. 1. Threshold voltages as a function of the ion concentration. Thin lines: $e > 0$, thick lines: $e < 0$. The values of e (in pC/m) are indicated at the curves

For very low ion content, $3\cdot10^{17}$ m^{-3}, the deformations are significant at one electrode and negligible at the other (curves 1 and 2). The director orientations vary gradually with the z coordinate. For $e < 0$, this distribution is due to the surface flexoelectric torques which are stabilizing at anode and destabilizing at cathode (curve 1). If $e > 0$, the torques have opposite signs (curve 2). The function $\theta(\zeta)$ for the positive e is equal to $\theta(-\zeta)$ for the negative e. This symmetry is due to symmetrical distribution of the electric field which is not perturbed by rather small ionic space charge.

For moderate ion content, $1\cdot10^{18} - 3\cdot10^{18}$ m^{-3}, similar director distribution arises in the upper voltage range for $e > 0$ (curve 3). In the lower voltage range, the deformation is significantly smaller (curve 4). For $e < 0$, the moderate ion content gives rise to the suppression of the deformation in the central part of the layer (curve 5).

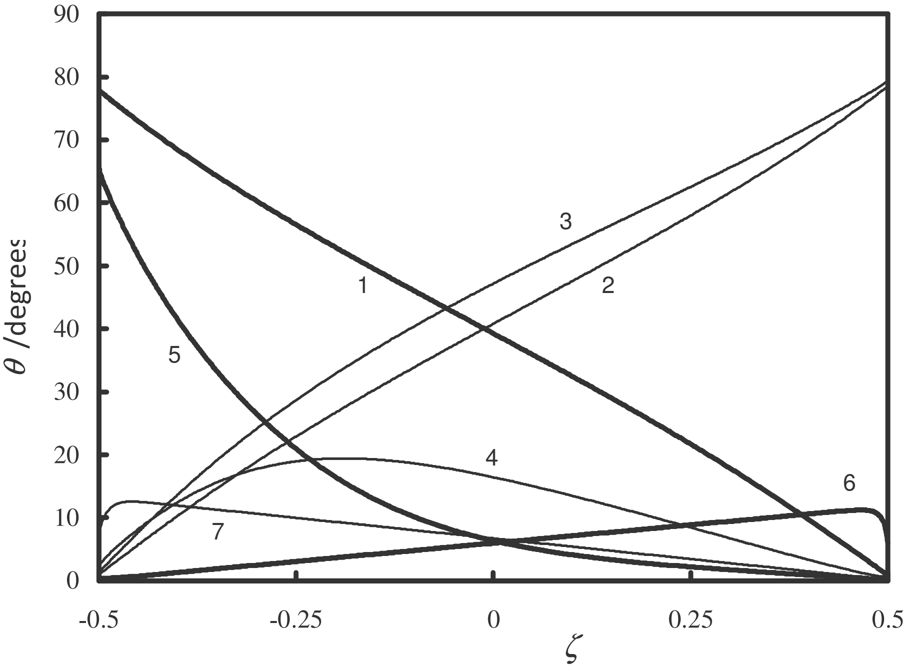

Fig. 2. Four kinds of director distributions for $e = 40$ pC/m (thin lines) and for $e = -40$ pC/m (thick lines). Curve 1: $N_0 = 3\cdot10^{17}$ m^{-3}, $U =$ 11.231 V; curve 2: $N_0 = 3\cdot10^{17}$ m^{-3}, $U =$ 11.253 V; curve 3: $N_0 = 10^{18}$ m^{-3}, $U =$ 11.242 V; curve 4: $N_0 = 3\cdot10^{18}$ m^{-3}, $U =$ 1.232 V; curve 5: $N_0 = 3\cdot10^{18}$ m^{-3}, $U =$ 10.241 V; curve 6: $N_0 = 10^{20}$ m^{-3}, $U = 0.968$ V; curve 7: $N_0 = 10^{20}$ m^{-3}, $U = 0.726$ V

For the highest ion concentrations, $N_0 = 10^{20}$ m^{-3}, the deformations are much weaker. The director distributions are determined by the very high surface fields and strong subsurface gradients. When $e < 0$, they lead to bulk flexoelectric destabilizing torque in the vicinity of the positive electrode and strong stabilizing torque in the neighbourhood of the negative electrode (curve 6). The stabilizing effect of the surface torque acting on the anode is also evident. The electric field in the prevailing part of the layer is homogeneous therefore it does not induce any torque. As a result, the angle describing the director orientation in this region varies almost linearly with the z coordinate. When $e > 0$, the torques have opposite senses (curve 7). In consequence, the function $\theta(\zeta)$ for the positive e is again approximately equal to $\theta(-\zeta)$ for the negative e.

5. SUMMARY AND DISCUSSION

In the present paper, the dielectrically compensated nematic possessing the flexoelectric properties was considered. This allowed us to study the role of the flexoelectric coefficients in the deformations of nematic layers. The results presented in this paper confirmed our earlier conclusions that the influence of flexoelectricity on the behaviour of the nematic layer strongly depends on the ion content. When the ion concentration exceeded c. $3{\cdot}10^{18}$ m^{-3}, the threshold voltage remarkably decreased below the theoretical value predicted for the insulating nematic. The larger mobility of anions than that of cations together with the negative sum of the flexoelectric coefficients cause arising of the additional low voltage range at which the deformations occur.

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] **Buczkowska M.**, **Machlowski M.**, Sci. Bull. Tech. Univ. Lodz, No. 1082, Physics, **31** (2010) 5.
[7] **Buczkowska M.**, Liq. Cryst., **37** (2010) 1331.
[8] **Buczkowska M.**, **Derfel G.**, Opto-Electronics Review, **19** (2011) 56.
[9] **Kashnow R.A.**, **Cole H.S.**, Mol. Cryst. Liq. Cryst., **23** (1973) 329.
[10] **Derzhanski A.**, **Petrov A.G.**, **Mitov M.D.**, J. Phys. (Paris), **39** (1978) 273.
[11] **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.
[12] **Derfel G.**, J. Mol. Liq., **144** (2009) 59.

DEFORMACJE WARSTW IZOTROPOWEGO DIELEKTRYCZNIE NEMATYKA FLEKSOELEKTRYCZNEGO WYWOŁANE STAŁYM POLEM ELEKTRYCZNYM

Streszczenie

Zbadano numerycznie wywołane polem elektrycznym odkształcenia warstw nematyków posiadających właściwości fleksoelektryczne, lecz pozbawionych anizotropii dielektrycznej. Obliczono napięcia progowe na odkształcenie. Wzięto pod uwagę niską, średnią i wysoką koncentrację jonów. Napięcia progowe przewidywane dla nematyków o wysokiej czystości sięgały 100 V. Napięcia progowe malały silnie ze wzrostem zawartości jonów. Określono także rozkłady direktora w warstwie. Wyróżniono cztery rodzaje rozkładów charakterystyczne dla niskiej, średniej i wysokiej koncentracji jonów.