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NUMERICAL STUDIES OF SIGNIFICANCE OF ANCHORING STRENGTH ENERGY FOR BEHAVIOUR OF FLEXOELECTRIC HOMEOTROPIC NEMATIC LAYER SUBJECTED TO DC ELECTRIC FIELD

Elastic deformations of homeotropic nematic liquid crystal layers subjected to a d.c. electric field were studied numerically. The flexoelectric properties of the nematic material and the presence of ionic space charge were taken into account. The influence of anchoring strength W was investigated. The calculations were performed for layers with negative dielectric anisotropy and negative sum of flexoelectric coefficients. Strongly blocking electrodes were assumed. The threshold voltages for deformations were computed for several anchoring strength values and for low, moderate and high ion content. Its value was nearly proportional to W for low anchoring strength and saturated at some high value of W. The director distributions were also determined. This task was complicated by the presence of space charge of ions. Remarkable change of deformation character was noticed when the ion content and anchoring strength were varied.

Keywords: flexoelectric nematic, anchoring strength; dc electric field induced deformations.

1. INTRODUCTION

Electric field-induced deformations of nematic layers arise as a result of torques exerted on the director in the bulk of the layer as well as at the surfaces. These torques are due to the dielectric anisotropy and flexoelectric properties of the nematic [1]. The flexoelectric contribution depends on the subsurface electric field strength which induces the surface torque, and on the electric field gradient which is responsible for the torque in the bulk. The dielectric torque is due to the electric field in the bulk. Therefore all the effects which influence the electric field distribution in the layer are significant. In particular, the deformations are affected by ions which are always present in liquid-crystalline materials. Therefore the ion space charge redistributed under the action of an external voltage is of great importance. When the boundary plates play the role of electrodes, and the surface alignment is strictly planar or homeotropic, deformations arise above some threshold voltage [1]. The form of the deformation results from the relationship between the magnitudes and signs of flexoelectric torques as well as from the magnitude and sign of the dielectric torque. It is also influenced by torques induced by the surface anchoring interactions which play a significant role.

In this paper we present results of calculations concerning the homeotropic layer of a nematic characterized by a negative sum of the flexoelectric coefficients and negative dielectric anisotropy subjected to d.c. electric field. We focused on the role of the anchoring strength in the deformations. The threshold voltages for deformations were computed for several values of anchoring strength and for low, moderate and high ion content. The director distributions were also determined. It was found that the effective influence of anchoring energy on deformations depends on the ion concentrations in liquid-crystalline material and therefore the ion content should be take into account during research of behaviour of nematic liquid crystals.

2. GEOMETRY AND PARAMETERS OF THE SYSTEM

The system under consideration was the same as that studied in previous papers [2-5]. The nematic liquid crystal was confined between two infinite plates which played the role of electrodes and were parallel to the *xy* plane and positioned at $z = \pm d/2$. A voltage U was applied between them. The lower electrode ($z = -d/2$) was earthed. The director **n** was parallel to the *xz* plane; its orientation was described by the angle $\theta(z)$, measured between **n** and the *z* axis. The material and layer parameters were as follows: thickness d = 20 μm, elastic constants $k_{11} = 6.2\times10^{-12}$ N and $k_{33} = 8.6\times10^{-12}$ N, the dielectric constant components $\varepsilon_{\parallel} = 4.7$ and $\varepsilon_{\perp} = 5.4$ which gives $\Delta\varepsilon = -0.7$, negative sum of the flexoelectric coefficients $e_{11}+e_{33} = -40\times10^{-12}$ Cm^{-1}. The homeotropic alignment was assumed. The anchoring strength was identical on both surfaces. It was determined by the Rapini-Papoular parameter W, [6], which was varied between 10^{-6} and 10^{-4} Jm^{-2}, for the extremely weak and for strong anchoring respectively.

The weak electrolyte model was adopted for the description of electrical phenomena in the layer [7,8]. The ion concentrations were determined by the generation constant β_0 and recombination constant α. In thermodynamic equilibrium, the ion concentration N_0 was equal to $\sqrt{\beta_0/\alpha}$. The value of dissociation constant, β_0 was varied from 10^{18} to 10^{21} $m^{-3}s^{-1}$. The resulting ion concentrations N_0 represented the low, moderate and high values of ion content and were of the order 10^{17}, 10^{18} and 10^{19} m^{-3} respectively. 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: $\mu_{\|}^{-} = 1.5\times10^{-9}$ $m^2V^{-1}s^{-1}$, $\mu_{\perp}^{-} = 1\times10^{-9}$ $m^2V^{-1}s^{-1}$, $\mu_{\|}^{+} = 1.5\times10^{-10}$ $m^2V^{-1}s^{-1}$, $\mu_{\perp}^{+} = 1\times10^{-10}$ $m^2V^{-1}s^{-1}$, i.e. $\mu_{\|}^{\pm}/\mu_{\perp}^{\pm} = 1.5$. The Einstein relation was assumed for the diffusion constants: $D_{\|,\perp}^{\pm} = (k_B T/q)\,\mu_{\|,\perp}^{\pm}$ 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 $D_{zz}^{\pm} = D_{\perp}^{\pm} + \Delta D^{\pm}\cos^2\theta$, respectively, where $\Delta\mu^{\pm} = \mu_{\|}^{\pm} - \mu_{\perp}^{\pm}$ and $\Delta D^{\pm} = D_{\|}^{\pm} - D_{\perp}^{\pm}$ denote the anisotropies of each quantity. The generation constant β depended on the electric field strength E: $\beta = \beta_0\left(1 + \dfrac{|E|q^3}{8\pi\varepsilon\,\bar{\varepsilon}\,k_B^2 T^2}\right)$, where $\bar{\varepsilon} = \left(2\varepsilon_{\perp} + \varepsilon_{\|}\right)/3$ and the recombination constant α, equal to 4.5×10^{-18} m^3s^{-1}, was calculated from the formula $\alpha = \dfrac{2q\bar{\mu}}{\varepsilon_0\varepsilon}$, where $\bar{\mu} = \left[\left(2\mu_{\perp}^{+} + \mu_{\|}^{+}\right)/3 + \left(2\mu_{\perp}^{-} + \mu_{\|}^{-}\right)/3\right]/2$ [9].

3. METHOD

The problem is considered to be one-dimensional. The reduced co-ordinate $\zeta = z/d$, is used in the following. The functions $\theta(\zeta)$, $V(\zeta)$ and $N^{\pm}(\zeta)$, which describe the director orientation, the potential and ions distribution within the layer, respectively, were determined by solving 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 [2].

The transport of ions in the bulk and across the electrode-liquid interfaces was described in terms of a model presented in details in the earlier papers [2,10]. The conducting properties of the layer are 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.

The threshold voltages U_T for the deformations were determined in the following way. The director distributions were calculated for several successively lowered voltages, including very small distortions, for which the maximum distortion angle θ_m was lower than 1º. The angle θ_m which was chosen as a measure of the deformation, was plotted vs. the voltage. No rapid decay of θ_m was detected, which indicated that the transition between the distorted and undistorted structures is of second order. The plots $\theta_m(U)$ were extrapolated to $\theta_m = 0$ which yielded the threshold voltage value with accuracy of 0.01 V. We find it sufficient for our purposes.

4. RESULTS

For given elastic constants, dielectric anisotropy and flexoelectric properties, the threshold voltage is influenced by the surface anchoring and the ion distributions which depend on the generation constant β_0, as well as on the properties of the electrodes. The threshold voltages for deformations were calculated for various anchoring strength W and for several coefficients β_0. The director distribution for voltages exceeding the thresholds by 0.1 V were also calculated in order to determine qualitative character of the deformations. The electric field distributions were also calculated. They can be useful for qualitative interpretation of the deformations.

4.1. Threshold voltage

For weak anchoring strength, the threshold U_T increases with W. For strong anchoring, the threshold becomes independent of W (Fig. 1). Such $U_T(W)$ dependence agrees qualitatively with theoretical formula derived for insulating nematic. The effect of ion content is shown in Fig. 2. For very weak anchoring, $W < 10^{-5}$ Jm^{-2}, the threshold decreases with ion content (determined by the dissociation constant β_0). For moderate value of anchoring strength,

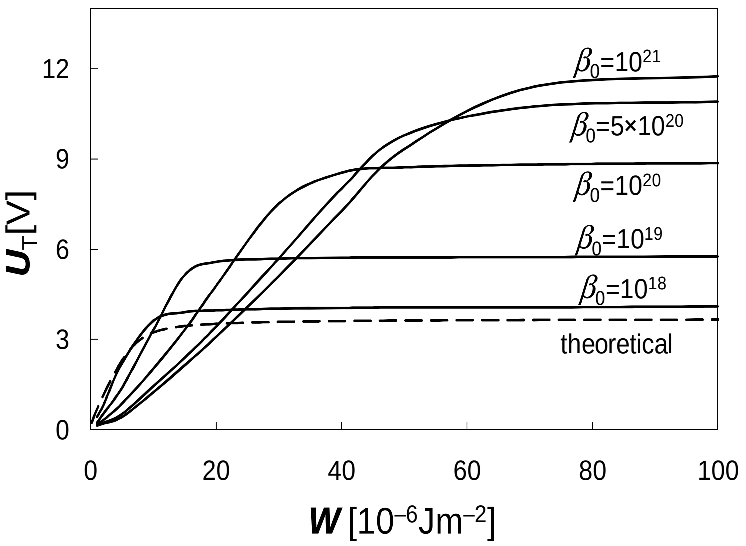

Fig. 1. Threshold voltages U_T as functions of anchoring strength *W* plotted for several dissociation coefficients β_0 indicated in $m^{-3}s^{-1}$ at the curves. The dashed line denotes the theoretical threshold calculated for an insulating nematic [1]

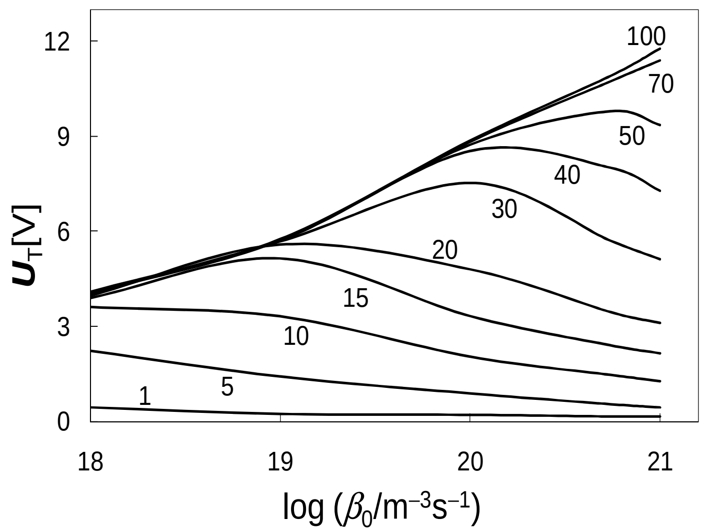

Fig. 2. Threshold voltages U_T as functions of dissociation coefficients β_0 plotted for several anchoring parameters *W* indicated in 10^{-6} Jm^{-2} at the curves

$W = 15 \div 50\times10^{-5}$ Jm^{-2}, there is a ion concentration at which the threshold voltage reaches a maximum. For rather rigid anchoring, $W > 50\times10^{-5}$ Jm^{-2}, the threshold increases monotonically with N_0.

4.2. Director distribution

Several types of director distributions in the deformed layer can be distinguished depending on the anchoring energy and ion content. They are illustrated in figures 3 – 6. They can be interpreted as a consequence of stabilizing or destabilizing torques of flexoelectric and dielectric origin induced by bias electric field, as it is illustrated in figure 7.

Figure 3 presents results for very low concentration, $N_0 = 4.7\times10^{17}$m^{-3}, corresponding to $\beta_0 = 10^{18}$ m^{-3}s^{-1}. For the cases of strong anchoring, (W = 70 and 100×10^{-6} Jm^{-2}), the deformation is limited to the bulk of the layer. It is due to prevailing destabilizing dielectric torque. The surface deformations are suppressed by the anchoring torques. For somewhat weaker anchoring, determined by W equal to 20 and 10×10^{-6} Jm^{-2}, the deformation is still dominated by the dielectric torque, but asymmetry of the director profile appears. At extremely weak anchoring (W = 1, 2 and 5×10^{-6} Jm^{-2}), the strong deformation occurs on the negative electrode and is negligible on the positive one. Such behaviour of the layer is related to predominant destabilizing surface flexoelectric torque acting on the left boundary. The bulk flexoelectric torques have minor significance due to relatively low electric field gradient (Fig. 8). The large deformation at $W = 5\times10^{-6}$ Jm^{-2} is somewhat surprising. This effect can be caused by the destabilizing surface flexoelectric torque which becomes enhanced with respect to the cases of $W = 1\times10^{-6}$ Jm^{-2} and $W = 2\times10^{-6}$ Jm^{-2} due to larger threshold voltage.

For a little higher ion content, i.e. $N_0 = 1.5\times10^{18}$ m^{-3} which corresponds to $\beta_0 = 10^{19}$ m^{-3}s^{-1} (Fig. 4), three significant changes of director profiles arising at weak anchoring can be noticed. For $W = 15\times10^{-6}$ Jm^{-2}, the deformation is the strongest and reaches the maximum in the left part of layer i.e. close to the negative electrode. The destabilizing dielectric torque plays still significant role and cooperates with the destabilizing surface flexoelectric torque acting at $z = d/2$. Effect of stabilizing surface torque is also visible in the thin subsurface region at the negative electrode. For $W = 5\times10^{-6}$ Jm^{-2} the deformation is practically limited only to left part of layer and is evidently due to the surface flexoelectric torque. For $W = 1\times10^{-6}$ Jm^{-2}, the deformation is governed by flexoelectric torques. In the case of the two latter anchoring strengths, the

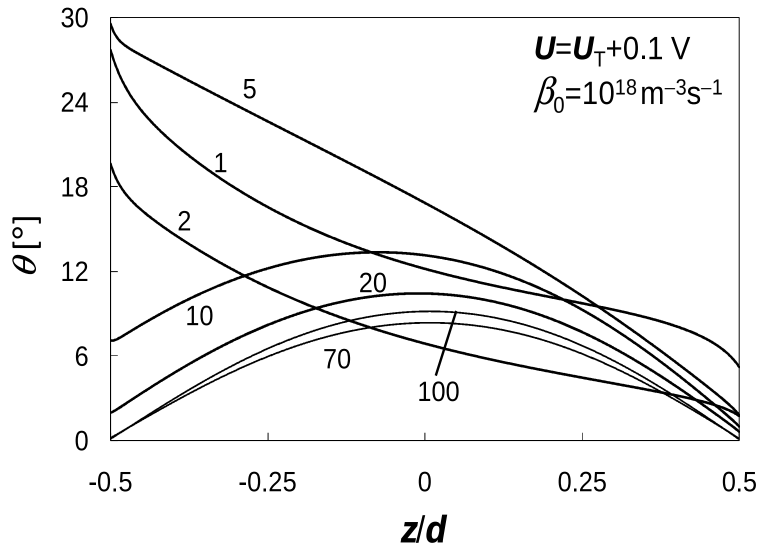

Fig. 3. Director distribution in the deformed layer presented by the angle $\theta(z/d)$ for several anchoring strength W in 10^{-6} Jm^{-2} indicated at the curves and for dissociation coefficient $\beta_0 = 10^{18}$m^{-3}s^{-1} corresponding to $N_0 = 4.7\times10^{17}$ m^{-3}

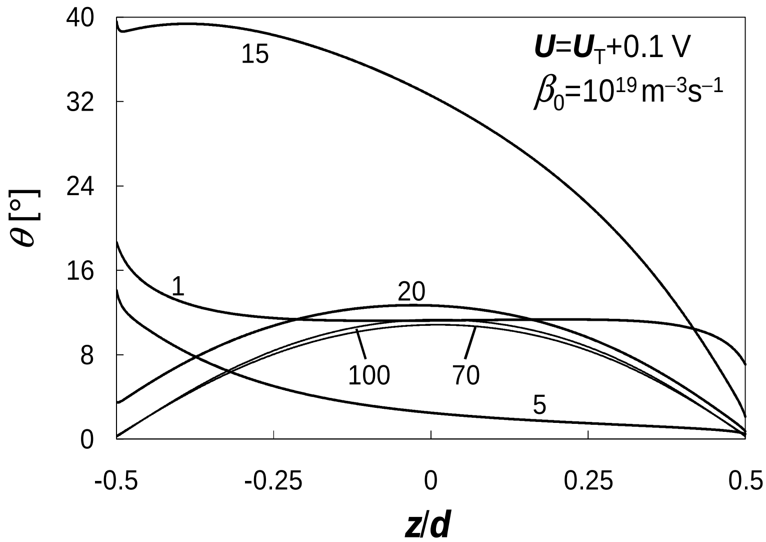

Fig. 4. Director distribution in the deformed layer presented by the angle $\theta(z/d)$ for several anchoring strength W in 10^{-6} Jm^{-2} indicated at the curves and for dissociation coefficient $\beta_0 = 10^{19}$ m^{-3}s^{-1} corresponding to $N_0 = 1.5\times10^{18}$ m^{-3}

deformation is somewhat weaker than in the layer with smaller ion concentration. This is due to stabilizing flexoelectric torque induced by the electric field gradient in the bulk (Fig. 9).

Figure 5 presents the results for the high ion content, $N_0 = 4.7\times10^{18}$ m^{-3}, which corresponds to $\beta_0 = 10^{20}$ m^{-3}s^{-1}. The director profile for $W = 15\times10^{-6}$ Jm^{-2} differs from the case of $\beta_0 = 10^{19}$ m^{-3}s^{-1}. The deformation is very small and limited to the left part of layer. For $W = 30\times10^{-6}$ Jm^{-2}, the deformation is stronger. The dielectric torque is compensated by the stabilizing bulk flexoelectric torque in the left half of the layer therefore the maximum of deformation is shifted to the vicinity of the negative electrode. The director profile for $W = 100\times10^{-6}$ Jm^{-2} is different from the profiles obtained for lower N_0. Its asymmetry is due to the stabilizing bulk flexoelectric torque which counteracts the dielectric torque. The surface deformations are suppressed by the anchoring interactions. The new form of director distributions appears also for weak anchoring ($W = 1$ and 5×10^{-6} Jm^{-2}). It is determined by the flexoelectric torques (as in the case of $W = 1\times10^{-6}$ Jm^{-2} shown in Fig. 4).

For sufficiently high ion concentration (Fig. 6), i.e. for $N_0 = 1.5\times10^{19}$ m^{-3} corresponding to $\beta_0 = 10^{21}$ m^{-3}s^{-1} and for small anchoring energy ($W = 2$, 5 and

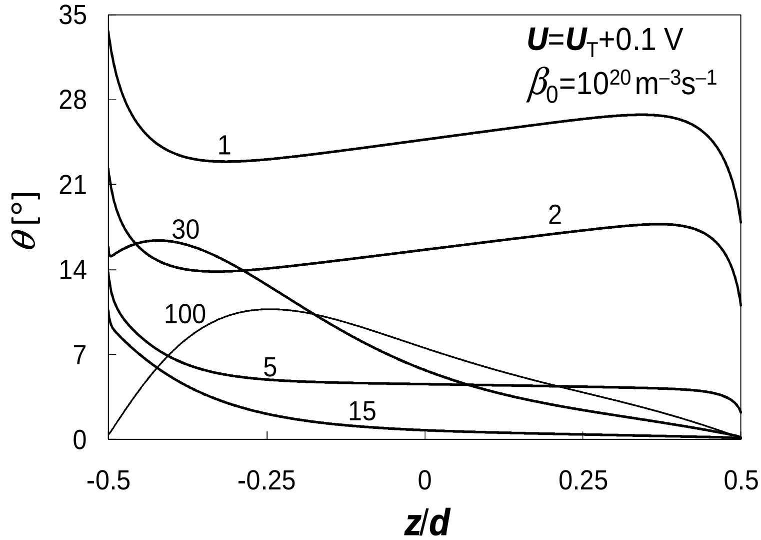

Fig. 5. Director distribution in the deformed layer presented by the angle $\theta(z/d)$ for several anchoring strength W in 10^{-6} Jm^{-2} indicated at the curves and for dissociation coefficient $\beta_0 = 10^{20}$ m^{-3}s^{-1} corresponding to $N_0 = 4.7\times10^{18}$ m^{-3}

$10{\times}10^{-6}\,\mathrm{Jm}^{-2}$), the same dominant role of flexoelectric torques is manifested. The deformation angle in the bulk increases linearly with the *z* co-ordinate. The deformation becomes stronger in vicinity of the negative electrode and decays close to the positive one. For $W = 50{\times}10^{-6}\,\mathrm{Jm}^{-2}$ the deformation is limited to the vicinity of the negative electrode. In the rest of layer the deformation disappears. For $W = 30{\times}10^{-6}\,\mathrm{Jm}^{-2}$, even weaker deformation is limited to narrow part of left half of the layer. In case of strong anchoring ($W = 100{\times}10^{-6}\,\mathrm{Jm}^{-2}$), the high ion content hardly affects the deformation in comparison with the case of $\beta_0 = 10^{20}\mathrm{m}^{-3}\mathrm{s}^{-1}$.

4.3. Electric field strength

The external voltage separates the ions and gathers them in the vicinity of the electrodes of opposite signs. In our case, (i.e. when the nematic has negative dielectric anisotropy and negative sum of flexoelectric coefficients), the dielectric torque plays destabilizing role in layer. The destabilizing surface torque acts at the negative electrode by contrast with stabilizing surface torque at the positive one. In the bulk, the stabilizing bulk flexoelectric torque acts in the prevailing part of layer. In the rest of layer the destabilizing bulk torque occurs.

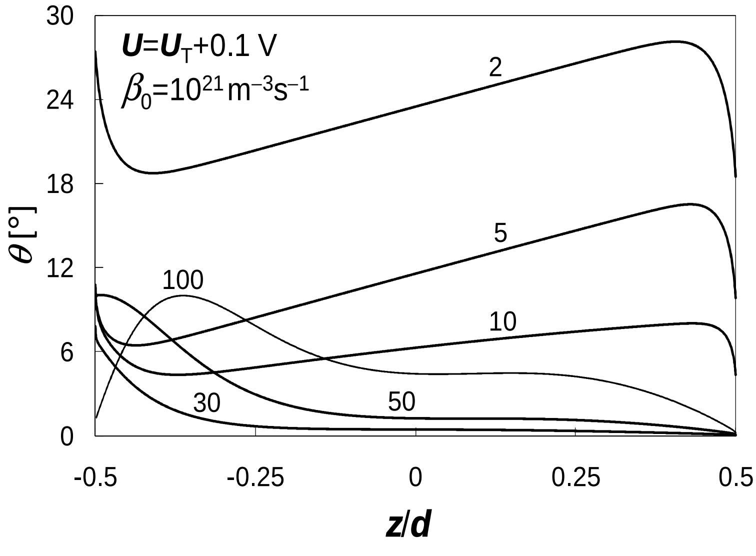

Fig. 6. Director distribution in the deformed layer presented by the angle $\theta(z/d)$ for several anchoring strength *W* in $10^{-6}\,\mathrm{Jm}^{-2}$ indicated at the curves and for dissociation coefficient $\beta_0 = 10^{21}\ \mathrm{m}^{-3}\mathrm{s}^{-1}$ corresponding to $N_0 = 1.5{\times}10^{19}\ \mathrm{m}^{-3}$

These effects of electric field are illustrated schematically in Fig. 7. The effectiveness of the torques depends not only on the field strength and field gradient values but also on the thickness of regions in which they act. The analysis and interpretation of the observed director profiles is therefore difficult and possible only ***a posteriori***.

In Figs. 8-11, the electric field strength distributions in the deformed layer are presented for several anchoring strengths *W* and for four dissociation coefficient β_0 corresponding to low, average and high ion content. The field strengths are calculated for $U = U_T + 0.1$ V, so it is obvious that their absolute values $|E|$ increase with anchoring energy ***W***. The electric field strength in the bulk is higher in left half of the layer than in the right half due to the difference between mobilities of anions and cations. This leads to field gradient which induces the stabilizing flexoelectric torque acting mainly in the left part of the layer.

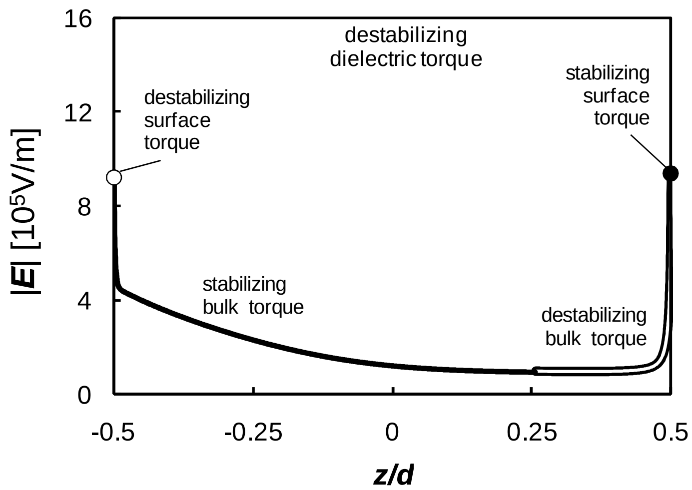

Fig. 7. Schematic presentation of stabilizing and destabilizing role of the flexoelectric torques acting in the bulk and on the surfaces for layer with negative dielectric anisotropy and negative sum of flexoelectric coefficients

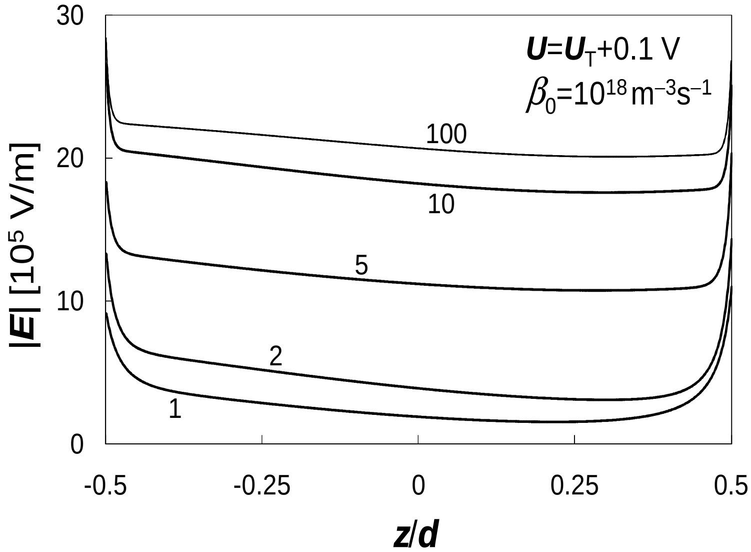

Fig. 8. Electric field strength distributions in the deformed layer presented for several anchoring strength W in 10^{-6} Jm^{-2} indicated at the curves and for dissociation coefficient $\beta_0 = 10^{18}\,\mathrm{m}^{-3}\mathrm{s}^{-1}$ corresponding to $N_0 = 4.7{\times}10^{17}\,\mathrm{m}^{-3}$

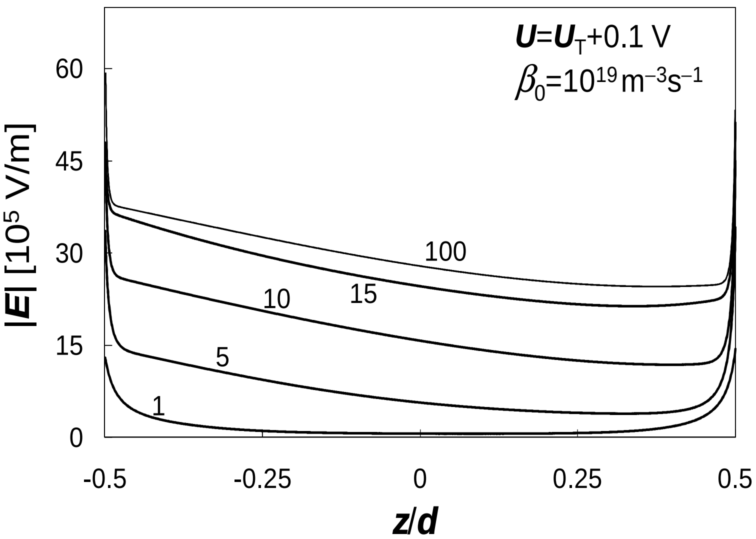

Fig. 9. Electric field strength distribution in the deformed layer presented for several anchoring strength W in 10^{-6} Jm^{-2} indicated at the curves and for dissociation coefficient $\beta_0 = 10^{19}\,\mathrm{m}^{-3}\mathrm{s}^{-1}$ corresponding to $N_0 = 1.5{\times}10^{18}\,\mathrm{m}^{-3}$

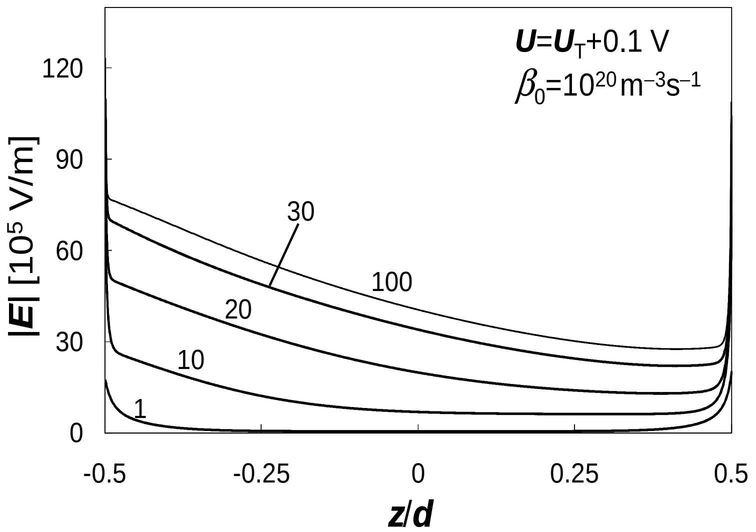

Fig. 10. Electric field strength distribution in the deformed layer presented for several anchoring strength W in 10^{-6} Jm^{-2} indicated at the curves and for dissociation coefficient $\beta_0 = 10^{20}$ $m^{-3}s^{-1}$ corresponding to $N_0 = 4.7\times10^{18}$ m^{-3}

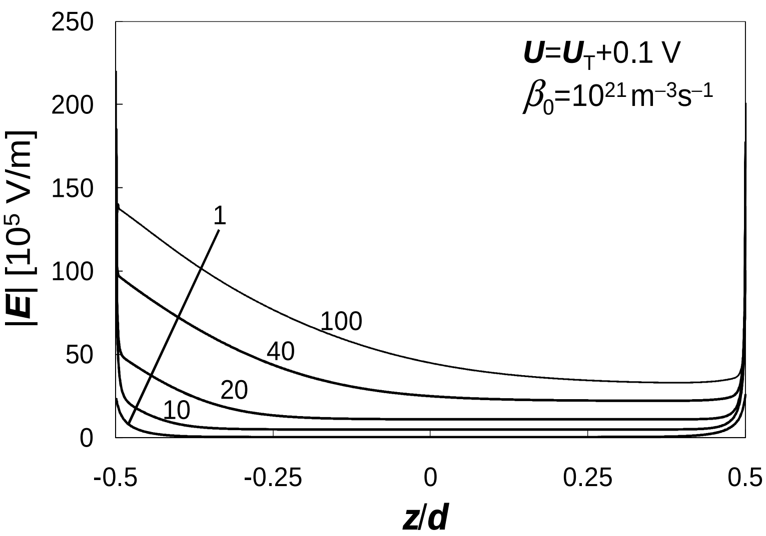

Fig. 11. Electric field strength distribution in the deformed layer presented for several anchoring strength W in 10^{-6} Jm^{-2} indicated at the curves and for dissociation coefficient $\beta_0 = 10^{21}$ $m^{-3}s^{-1}$ corresponding to $N_0 = 1.5\times10^{19}$ m^{-3}

5. CONCLUSIONS

The influence of anchoring energy on the deformations should be considered together with the influence of the ionic space charge. Stabilizing effect of anchoring torques can be reduced by the influence of the space charges of ions accumulated at the electrodes which generate strong electric fields on the boundaries and high electric field gradients in the subsurface regions. Similar conclusion was drawn from theoretical considerations made in [11] where the need of renormalization of the anchoring energy due to ions was found.

The subsurface bulk torques and surface torques can overcome the anchoring torques. As a consequence, for a particular director distribution observed for given values of W and N_0, one can find a qualitatively similar director profile occurring for somewhat stronger anchoring and higher ion content. This effect is exemplified by the curves for $W = 5$, 15 and 30×10^{-6} Jm^{-2} in Figs. 4, 5 and 6 respectively.

Difference of mobility of anions and cations causes asymmetry of the electric field distribution and gives rise to asymmetry of the director deformations in addition to the flexoelectric torques.

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NUMERYCZNE BADANIA WPŁYWU ENERGII KOTWICZENIA NA ODKSZTAŁCENIA HOMEOTROPOWEJ WARSTWY NEMATYKA FLEKSOELEKTRYCZNEGO WYWOŁANE STAŁYM POLEM ELEKTRYCZNYM

Streszczenie

Zbadano numerycznie wpływ energii kotwiczenia ciekłego kryształu z podłożem na indukowane stałym polem elektrycznym deformacje homeotropowej warstwy nematyka o ujemnej anizotropii dielektrycznej i ujemnej sumie współczynników fleksoelektrycznych. Przy niskiej zawartości jonów i wysokiej energii kotwiczenia stwierdzono symetryczny rozkład direktora. W miarę wzrostu koncentracji jonów lub obniżania energii kotwiczenia deformacja stawała się asymetryczna. Wyniki pokazują, że jonowy ładunek przestrzenny wpływa znacząco na efektywność oddziaływań powierzchniowych.