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INFLUENCE OF TILTED SURFACE ALIGNMENT ON FLEXOELECTRIC DOMAINS IN TWISTED NEMATIC LAYERS

The small deformations induced by electric field in twisted flexoelectric nematic layers were simulated numerically. The one-dimensional (i.e. homogeneous over the whole area of the layer) and two-dimensional (i.e. spatially periodic flexoelectric domains) deformations were considered. It was shown that the periodic deformations do not arise if sufficiently high pretilt angle is imposed by the boundary conditions. The value of pretilt angle necessary for elimination of domains increases with the flexoelectric coefficient e_{33}. This result is of practical meaning because the flexoelectric domains are undesirable from an applicative point of view since they destroy the homogeneous appearance of the area of an excited pixel of a display.

Keywords: nematics; flexoelectricity; director deformations; periodic patterns.

1. INTRODUCTION

Nematic liquid crystal layers confined between plane-parallel electrodes are fundamental for applications in liquid crystal devices [1]. The principle of operation of these devices is based on electrically induced deformations of director field. The deformations arise due to torques of dielectric and flexoelectric nature [2]. They can be one-dimensional or two-dimensional. In the former case the director orientation depends on the coordinate z perpendicular to the layer plane only. In the latter case, the director orientation depends on z and varies periodically along another direction parallel to the layer. As a result, the deformation is spatially periodic and is visible in the form of parallel stripes called domains [3-5]. The two-dimensional deformations are particularly favoured if nematic possesses significant flexoelectric properties which was demonstrated in our earlier article [6]. Nematic exhibiting strong flexoelectricity adopted enhanced interest after they were discovered among substances composed of molecules with bent core [7, 8]. The flexoelectric domains are not desirable from applicative point of view since they disturb the uniform appearance of an excited pixel of a device. However, in our previous article [9] we showed that they can be avoided if the boundary conditions ensure sufficiently large surface pretilt of easy axes which determine orientation of director adjacent to the electrodes.

In the present paper we continue the calculations taking into account the nematics which exhibit parameters characteristic for the mixtures of substances composed of calamitic and bent-core molecules.

2. PARAMETERS AND METHOD

The nematic layers of thickness $d = 5$ μm, confined between electrodes parallel to the xy plane of the coordinate system and positioned at $z = \pm d/2$, were considered. The voltage U was applied between them. The director orientation in the layer, $\mathbf{n}(y,z)$, was determined by means of the polar angle $\theta(y,z)$ measured between $\mathbf{n}$ and the xy plane and by the azimuthal angle $\phi(y,z)$ between the x axis and the projection of $\mathbf{n}$ on the xy plane. Boundary conditions were given by the polar and azimuthal angles θ_{s1}, θ_{s2}, ϕ_{s1} and ϕ_{s2} which determined orientation of the easy axes $\mathbf{e_1}$ and $\mathbf{e_2}$ on the lower and upper electrode, respectively. The surface pretilt angles $\theta_{s1} = \theta_{s2}$, in the following denoted by δ, ranging between 0° and 30°, were imposed. The twist angle $\Phi = \phi_{s2} - \phi_{s1} = 90°$ ensured the right-hand twist in the twisted layers. The calculations were performed for two kinds of mixtures denoted in the following as mixtures A and mixtures B. The bent-core nematics have peculiar elastic properties manifested by the specific relation between elastic constants: $k_{11} > k_{33} > k_{22}$ [10]. For this reason we adopted elastic constants ratios which differ from those found for typical calamitic nematics. The parameters of the corresponding layers are gathered in Table 1.

Table 1

The parameters of the layers

	mixtures A	mixtures B
splay elastic constants	$k_{11} = 8\cdot10^{-12}$ N	$k_{11} = 7\cdot10^{-12}$ N
twist elastic constants	$k_{22} = 3\cdot10^{-12}$ N	$k_{22} = 2\cdot10^{-12}$ N
bend elastic constants	$k_{33} = 10\cdot10^{-12}$ N	$k_{33} = 7\cdot10^{-12}$ N
dielectric anisotropy	$\Delta\varepsilon = 2$	$\Delta\varepsilon = 2$
bend flexoelectric coefficient	0 - $50\cdot10^{-12}$ C/m	0 - $50\cdot10^{-12}$ C/m
polar anchoring strength	$W_{\theta1} = W_{\theta2} = 10^{-4}$ J/m^2	$W_{\theta1} = W_{\theta2} = 10^{-4}$ J/m^2
azimuthal anchoring strength	$W_{\phi1} = W_{\phi2} = 10^{-5}$ J/m^2	$W_{\phi1} = W_{\phi2} = 10^{-5}$ J/m^2

The splay flexoelectric coefficient e_{11} was assumed to be zero since the role of the bend flexoelectric coefficient e_{33} is predominant in bent-core materials. Its value was varied between 0 and 50 pC/m. The saddle-splay elastic constant k_{24} was assumed to be zero. The small dielectric anisotropy of the mixtures was adopted according to small positive or negative values measured for the bent-core nematics. Such small dielectric anisotropy only slightly influenced the effects of flexoelectric nature which were our main interest.

We simulated both the small one-dimensional deformations as well as the small periodic deformations after application of voltage. The director distribution along the z axis was found in the former case and the distribution in the cross-section of a single stripe was determined in the latter case. The method of computations was comprehensively described in our previous paper [9]. The equilibrium director distribution was found by minimisation of free energy per unit area of the layer at the bias voltage which caused small deformation. The state of minimum energy was obtained in the course of an iteration process. During a single cycle of computations, the variables describing the director distribution were varied successively by small intervals. The free energy per unit area of the layer was calculated after each change. If the new energy was lower than the previous one, the changed values of the variables were accepted. In the opposite case, the variables remained unchanged and another attempt was made. The cycles were repeated until further reduction in the total free energy could be neglected. The energies per unit area of the layer calculated for one-dimensional and two-dimensional deformations arising at the same voltage were compared. The state with lower energy was chosen as the one which is realized. The calculations were performed for increasing voltages starting from $U = 0$. The threshold voltage for the periodic deformations, U_c, was determined as the voltage at which the energy of them became smaller than that for homogeneous deformations.

2. RESULTS

In the case of layers with zero pretilt, the spatially periodic deformations arose when the threshold voltage U_0 was exceeded. The layers with non-zero pretilt started to deform homogeneously already from $U = 0$. The two-dimensional deformations appeared at the threshold voltage U_c on the background of the small homogeneous deformation. The threshold voltage decreased with increasing flexoelectric coefficient e_{33}. For given value of e_{33} the threshold increased when the pretilt angle was enhanced. Both dependences are presented for the mixtures A and B in Figs. 1 and 2 respectively, where thresholds U_c are plotted as functions of pretilt angle δ for several values of e_{33}.

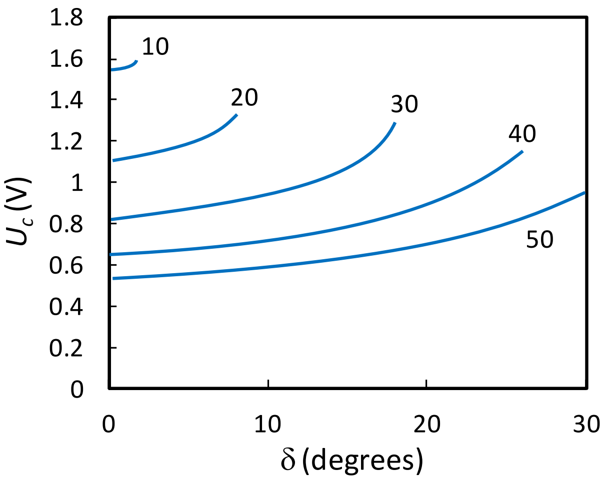

Fig. 1. Threshold voltage U_c as a function of surface pretilt angle δ for mixtures A. Values of flexoelectric coefficients e_{33} (in pC/m) are indicated at the curves

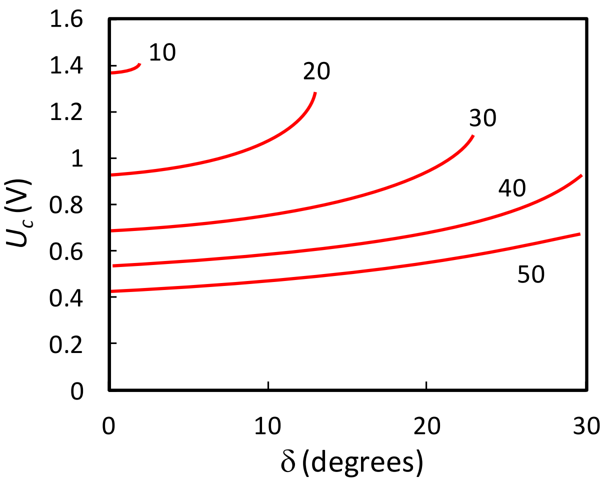

Fig. 2. Threshold voltage U_c as a function of surface pretilt angle δ for mixtures B. Values of flexoelectric coefficients e_{33} (in pC/m) are indicated at the curves

It is evident that for the weakly flexoelectric nematics there exist some critical pretilt angles δ_c above which the periodic deformations are no more energetically favoured therefore they do not occur. This means that the flexoelectric domains are eliminated. In the case of strongly flexoelectric mixture the critical pretilt exceeds 30°. However we restricted our calculations to this value since larger pretilt angles seem to be impractical.

The results are summarised in Fig. 3. they are coherent with those reported in [9]. The plots of the critical pretilt angle as a function of flexoelectric coefficient limit the set of parameters δ and e_{33} for which the flexoelectric domains are favoured from the set for which the domains are eliminated.

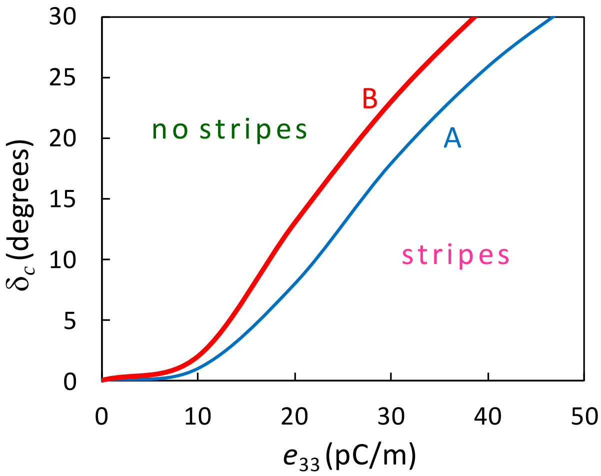

Fig. 3. Limiting pretilt angle δ_c as a function of flexoelectric coefficient e_{33} for mixtures A and B

The results of this work show that the sufficiently large surface pretilt angle allows to avoid the flexoelectric domains when the nematic material possesses strong flexoelectric properties.

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WPŁYW UKOŚNEGO UPORZĄDKOWANIA POWIERZCHIOWEGO NA DOMENY FLEKSOELEKTRYCZNE W SKRĘCONYCH WARSTWACH NEMATYKA

Streszczenie

Niewielkie odkształcenia wywołane polem elektrycznym w warstwach skręconego nematyka były symulowane numerycznie. Badano odkształcenia jednowymiarowe (tj. jednorodne na całej powierzchni warstwy) i dwuwymiarowe (tj. przestrzennie okresowe). Wykazano, że odkształcenia okresowe nie powstają, gdy warunki brzegowe narzucają odpowiednio duży kąt nachylenia uporządkowania powierzchniowego. Jego wartość rośnie ze wzrostem współ-czynnika fleksoelektrycznego e_{33}. Wynik ten ma znaczenie praktyczne, ponieważ występowanie domen fleksoelektrycznych w urządzeniach ciekłokrystalicznych jest niepożądane.