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INFLUENCE OF CHIRALITY ON TWO-DIMENSIONAL DEFORMATIONS IN TWISTED FLEXOELECTRIC NEMATIC LAYERS

Two-dimensional deformations induced by electric field in twisted nematic cells filled with liquid crystal possessing flexoelectric properties were simulated numerically. The influence of chiral dopants on the occurrence and structure of the spatially periodic patterns was investigated. It was found that the chirality influences mainly the direction of the periodic patterns whereas the threshold voltage for deformation and the width of the stripes are weakly affected.

Keywords: twisted nematic, flexoelectricity, chirality, periodic patterns.

1. INTRODUCTION

Thin layers of nematic liquid crystals confined between plane-parallel electrodes are fundamental for construction of displays and of other liquid crystal devices [1]. The twisted nematic cells in which the undistorted director remains parallel to the boundary plates but is twisted by $\Phi = 90^{\circ}$ along the normal to the layer are the most common. The structure twisted by 90° is achieved due to suitable surface anchoring which determines the easy axes oriented in mutually crossed directions. The twisted structure arises if the layer is filled with pure nematic material or if it is doped with some chiral substance which imposes some intrinsic pitch *p*. The chirality, defined as $q = 2\pi/p$, should range between 0 and $\pi/(2d)$. In the latter case, the intrinsic pitch is compatible with the twist angle Φ .

General principle of operation of the twisted nematic cells consists in electric field induced deformations of director orientation. Two kinds of distortions are possible: one-dimensional, *i.e.* homogeneous over the whole area of the electrodes and two-dimensional in which the director orientation depends

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not only on the coordinate normal to the layer but it also varies along some direction parallel to the layer [2, 3]. The two-dimensional deformations are spatially periodic. They are visible under microscope in the form of parallel stripes. They also destroy homogeneous appearance of the area of an excited pixel of a display, therefore are undesirable.

The influence of electric field on director distribution is due to dielectric anisotropy and to flexoelectricity of the nematic material [4, 5]. The occurrence of one- and two-dimensional deformations induced in pure nematic substance (q = 0) was studied in the earlier paper [3, 6]. It was found that if the nematic possesses sufficiently strong flexoelectric properties, then the spatially periodic deformations. This is interesting because flexoelectricity can become essential feature of a nematic mixture if it contains mesogenic substances composed of bent-core molecules which exhibit giant flexoelectric properties [7, 8]. The stripes are characterized by their width λ and by the angle ψ which they make with the direction of the mid-plane director orientation in the undistorted structure. Two types of stripes were distinguished which differ in structure and direction [3].

The aim of the present paper is to study the role of chirality for arising of the stripes. Various values of the chirality were taken into account.

2. ASSUMPTIONS AND METHOD

The nematic structure of thickness $d = 6 \,\mu\text{m}$ confined between two plane electrodes parallel to the *xy* plane of Cartesian coordinate system positioned at $z = \pm d/2$ and twisted by $\Phi = 90^{\circ}$ was considered. We assumed that all the physical quantities and variables describing the two dimensional structures depended on two coordinates, *y* and *z*, and were constant along the *x* axis. The director orientation $\mathbf{n}(y,z)$ was determined by means of the polar angle $\theta(y,z)$ measured between **n** and the *xy* plane and by the azimuthal angle $\phi(y,z)$ made between the *x* axis and the projection of **n** on the *xy* plane. Voltage *U* was applied between the electrodes. The lower electrode was earthed, *i.e.* potential V(-d/2) = 0. Boundary conditions were determined by the polar and azimuthal angles $\theta_{s1} = \theta_{s2} = 0$, $\phi_{s1} = -45^{\circ}$ and $\phi_{s2} = 45^{\circ}$ which determined orientation of the easy axes $\mathbf{e_1}$ and $\mathbf{e_2}$ on the lower and upper electrode, respectively. The anisotropic surface anchoring, expressed by the formula proposed in [9], was assumed. The anchoring energy was determined by polar and azimuthal anchoring strengths, $W_{\theta 1} = W_{\theta 2} = 10^{-4} \text{ J/m}^2$, $W_{\phi 1} = W_{\phi 2} = 10^{-5} \text{ J/m}^2$. The elastic



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constants of the nematic were $k_{11} = 8$ pN, $k_{22} = 3$ pN, $k_{33} = 10$ pN. Small positive dielectric anisotropy $\Delta \varepsilon = 2$ was assumed. Flexoelectric properties were defined by the bend flexoelectric coefficient $e_{33} = 20$ pC/m, while the splay coefficient e_{11} was set to zero, which reflected the features of mixtures containing the bent-core nematic substance. The presence of ions was neglected, *i.e.* the nematic was treated as perfect insulator. The equilibrium structures of the director field inside the layer were determined by minimization of the free energy counted per unit area of the layer. For this purpose, we used the method which was successfully applied in earlier works [3]. The electric potential distribution V(y,z) in the layer was calculated by resolving the Poisson equation.

3. RESULTS

The results of computations are coherent with earlier data found for nonchiral flexoelectric nematic layers [3]. The two-dimensional deformations arose at some threshold voltage U_1 as shown in Fig. 1 where the maximum polar orientation angle θ_{max} was used as a measure of deformation. The deformation took the form of periodic pattern denoted as the stripes of type 1. Their energy was lower than the energy of simulated one-dimensional deformations.



Fig. 1. Maximum polar orientation angle in two-dimensional deformation (solid lines) and in simulated one-dimensional deformation (dashed line) as functions of bias voltage. The arrows show the evolution of deformation during increase and decrease of voltage; $q = 0.065 \ \mu m^{-1}$.

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The threshold U_1 was smaller than the threshold for uniform deformations. The width of the stripes was initially several times larger than thickness of the layer and decreased with voltage as shown in Fig. 2. Direction of the stripes was determined by the angle ψ ranging between -40° and 0° which varied with voltage (Fig. 3).



Fig. 2. Space period of the two-dimensional deformation as a function of bias voltage. The arrows show the evolution of deformation during increase and decrease of voltage; $q = 0.196 \ \mu m^{-1}$.



Fig. 3. Direction of the two-dimensional deformations as a function of bias voltage. The arrows show the evolution of deformation during increase and decrease of voltage; 1: q = 0; 2: $q = 0.065 \mu m^{-1}$; 3: $q = 0.131 \mu m^{-1}$; 4: $q = 0.196 \mu m^{-1}$; 5: $q = 0.262 \mu m^{-1}$.



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The second type of the periodic deformations, denoted as type 2, appeared discontinuously at some higher threshold U_2 . The type 2 stripes differed from the type 1 in director distribution, in their width and direction. Figure 1 shows that the type 2 deformations developed with increasing voltage and that they were retained if the bias voltage was decreased below U_2 . At some another critical voltage U_3 , the width of the type 2 stripes diverged to infinity leading to one-dimensional deformations (Fig. 2). However, the most peculiar effect revealed during simulations was the significant change of direction of the stripes during transition from type 1 to type 2 presented in Figs. 3 and 4.



Fig. 4. Directions of the type 1 and type 2 stripes at $U = U_2$.

The scheme of evolution of the stripes described above was found for any value of chirality.

Exemplary director distributions in the cross-sections of single stripes of both types are presented in Fig. 5 for the case of chirality compatible with the 90° twist, $q = 0.262 \ \mu m^{-1}$. Slight difference between both distributions can be noticed in the vicinity of the lower electrode where the disclination lines were created. The chirality weakly affected the structure of the deformed layer but it influenced significantly the directions of the periodic patterns. The angle ψ was decreased by c. 15° when the chirality was varied from zero to $q = 0.262 \ \mu m^{-1}$ (Fig. 5). In the latter case, the angle ψ for the stripes of type 2 was equal to 45° in agreement with results presented in [3]. The width of the stripes was weakly affected by the chirality. The same concerned the characteristic voltages U_1 , U_2 and U_3 (Fig. 6). The threshold voltage for deformations, U_1 , as well as the value of U_3 were practically constant. The voltage for arising of type 2 deformation, U_2 , slightly increased with chirality. M. Buczkowska



Fig. 5. Director distributions in the cross-sections of single stripes of type 1 (top) and type 2 (bottom), U = 3 V, $q = 0.262 \text{ }\mu\text{m}^{-1}$.

4. SUMMARY

The nematic layer twisted by 90° can be obtained with use of pure nematic as well as with use of substances containing dopants inducing chirality q ranging from zero to 0.262 μ m⁻¹. In each case, the periodic patterns in the form of stripes arose under the action of external electric field. Two types of stripes were observed. It was found that the chirality influences mainly the direction of the periodic patterns whereas the threshold voltage for deformation and the width of the stripes are weakly affected.





Fig. 6. Characteristic voltages as functions of chirality.

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WPŁYW CHIRALNOŚCI NA DWUWYMIAROWE ODKSZTAŁCENIA WARSTW NEMATYKÓW FLEKSOELEKTRYCZNYCH

Streszczenie

Dwuwymiarowe deformacje indukowane polem elektrycznym w warstwach ciekłych kryształów nematycznych posiadających właściwości fleksoelektryczne były symulowane numerycznie. Zbadano wpływ chiralnych domieszek na strukturę tych odkształceń i ich rozwój pod wpływem pola elektrycznego. Stwierdzono, że chiralność wpływa głównie na kierunek odkształceń, podczas gdy napięcie progowe na odkształcenie i przestrzenny okres odkształceń słabo zależą od chiralności nematyka.

Stwierdzono, że chiralność wpływa głównie na kierunek odkształceń, podczas gdy jej wpływ na napięcie progowe i na przestrzenny okres odkształceń jest nieznaczny.