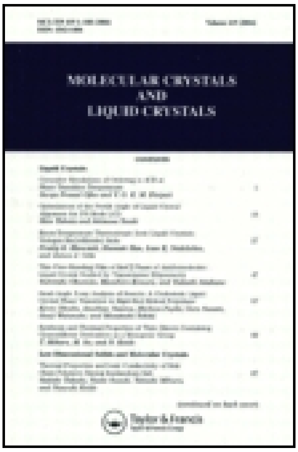

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Numerical Study of Flexoelectric Longitudinal Domains

G. Derfel [a] & M. Buczkowska [a]
[a] Institute of Physics, Technical University of Łódź, Łódź, Poland

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Numerical Study of Flexoelectric Longitudinal Domains

G. DERFEL AND M. BUCZKOWSKA

Institute of Physics, Technical University of Łódź, Łódź, Poland

The role of flexoelectric properties in arising of the electric field induced periodic deformations of nematic planar layers, known as longitudinal domains, was determined numerically. Rigidly anchored insulating nematic was considered. Both signs of dielectric anisotropy were taken into account. The structure of the domains was determined. The threshold voltages for arising of the domains and their initial spatial period were calculated as functions of dielectric anisotropy and of elastic constants ratio k_{22}/k_{11}, *for various values of the difference of flexoelectric coefficients* $|e_{11} - e_{33}|$. *The ranges of these parameters, for which the domains exist, were determined.*

Keywords Flexoelectric properties; longitudinal domains; periodic deformations

1. Introduction

Deformations of director distribution in nematic layers induced by external fields can have twofold character. Let us consider a nematic liquid crystal layer confined between two infinite plates parallel to the xy plane of the Cartesian coordinate system. The angles which determine the director orientation can vary along one coordinate z perpendicular to the layer plane or along two coordinates, z and, for example, y. In the latter case, the distorted director field takes the form of periodic pattern visible under the polarising microscope as stripes. The periodic deformation can be characterised by the wave vector $\mathbf{q}$ of length $q = |\mathbf{q}| = 2\pi/\Lambda$, where Λ is the spatial period of the structure. The periodic patterns, both static and transient, were detected in various configurations of external field and initial director alignment, in the magnetic as well as in the electric field and were analysed theoretically [1–3]. The comprehensive review of the periodic patterns of various natures was given by Hinov *et al.* [4].

The deformations of nematic liquid crystal layers induced by external electric field are due to the dielectric anisotropy as well as to the flexoelectric properties of the liquid crystalline medium. The periodic deformations appear if the free energy per unit area of the layer connected with them is lower than the free energy due to the one-dimensional deformation which would arise under the same circumstances. Such relationship occurs only when the parameters of the system satisfy suitable conditions. One can distinguish five elementary configurations of electric field vector

Address correspondence to G. Derfel, Institute of Physics, Technical University of Łódź, ul. Wólczańska 219, 90-924 Łódź, Poland. E-mail: gderfel@p.lodz.pl

E and initial director alignment $\mathbf{n_0}$ in which the static periodic deformations can be expected. In particular, some kind of the periodic deformations was discovered by Vistin [5] in the planar layer, $\mathbf{n_0} = (1, 0, 0)$, subjected to the field $\mathbf{E} = (0, 0, E)$ and with the wave vector $\mathbf{q} = (0, 1, 0)$. They were attributed to flexoelectric properties of the nematic material [6] and are called Vistin domains or longitudinal domains. They were also analysed theoretically [7,8].

The aim of the present paper is to determine numerically the role of the flexoelectric properties in appearance of the Vistin domains. Insulating nematic was considered. Rigid boundary anchoring was assumed. Both signs of dielectric anisotropy $\Delta\varepsilon$ were taken into account. The calculations allowed to verify earlier results obtained theoretically in linear approximation and with assumption of equal elastic constants. It was confirmed that the influence of flexoelectric properties depends on the difference of the flexoelectric coefficients, $\Delta e = |e_{11} - e_{33}|$. The threshold voltages U_0 for arising of periodic deformations and the initial spatial period Λ_0 of the periodic patterns were calculated as functions of dielectric anisotropy $\Delta\varepsilon$ and of elastic constants ratio $r = k_{22}/k_{11}$ for various values of flexoelectric parameter Δe. The structure of the stripes was recognized. The ranges of $\Delta\varepsilon$, Δe and r for which the patterns exist, were determined.

2. Assumptions, 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 played the role of electrodes. The voltage U was applied between them; the lower electrode ($z = \pm d/2$) was earthed. Rigid planar alignment identical on both boundary plates, was assumed. The director orientation was described by the angle $\theta(y, z)$, measured between **n** and the xy plane and by the angle $\varphi(y, z)$, measured between projection of **n** on the xy plane and the x axis. The model substance was characterized by the elastic constants $k_{11} = 6.2 \times 10^{-12}\,\mathrm{N}$ and $k_{33} = 8.6 \times 10^{-12}\,\mathrm{N}$. The k_{22} elastic constant was determined by the ratio $r = k_{22}/k_{11}$ which was varied from 0.2 to 1. The dielectric anisotropy $\Delta\varepsilon$ was varied between -10 and $+20$. The flexoelectric properties were expressed by the absolute value of the difference of flexoelectric coefficients $\Delta e = |e_{11} - e_{33}|$ which was varied from 0 to $20 \times 10^{-12}\,\mathrm{Cm}^{-1}$ (the separate values of e_{11} and e_{33} are not essential in the considered geometry in agreement with [7]). The nematic was assumed to be insulating, which corresponded to highly purified material.

3. Method

A single stripe of width Λ was considered. The director orientation over the cross section of the stripe described by the angles $\theta(y, z)$, and $\varphi(y, z)$ was approximated by their most significant Fourier components satisfying the rigid anchoring and periodic boundary conditions along y:

$$\theta(y,z) = [A\cos(\pi z/d) + B\sin(2\pi z/d)]\cos(2\pi y/\Lambda) + D\cos(\pi z/d) + F\sin(2\pi z/d) \tag{1}$$

$$\phi(y,z) = [G\cos(\pi z/d) + H\sin(2\pi z/d)]\sin(2\pi y/\Lambda) \tag{2}$$

Such approach is often used in theoretical analyses [9,10]. It describes properly small distortions and ensures correct values of the threshold voltages for periodic deformations whenever they exist. The last two components in Eq. (1) express a possibility of arising of the one-dimensional deformations.

The structure of the stripe was found by numerical minimization of the free energy per unit area of the layer given by the formula

$$g = \frac{1}{\Lambda L} \int_{-d/2}^{d/2} \int_{0}^{\Lambda} \int_{0}^{L} (g_{elastic} + g_{dielectric} + g_{flexoelectric}) \mathrm{d}x\mathrm{d}y\mathrm{d}z \tag{3}$$

where

$$g_{elastic} = (1/2)k_{11}(\nabla \cdot \mathbf{n})^2 + (1/2)k_{22}[\mathbf{n} \cdot (\nabla \times \mathbf{n})]^2 + (1/2)k_{33}[\mathbf{n} \times (\nabla \times \mathbf{n})]^2 \tag{4}$$

$$g_{dielectric} = -(1/2)\varepsilon_0 \Delta\varepsilon (\mathbf{E} \cdot \mathbf{n})^2 \tag{5}$$

$$g_{flexoelectric} = -[e_{11}\mathbf{n}(\nabla \cdot \mathbf{n}) - e_{33}\mathbf{n} \times (\nabla \times \mathbf{n})]\mathbf{E} \tag{6}$$

and L is an arbitrary length along the x axis. The electric field strength was uniform, $\mathbf{E} = (0, 0, E)$, according to the assumption of small deformations.

The continuous functions $\theta(y, z)$ and $\varphi(y, z)$ given by Eqs. (1) and (2) were replaced by discrete angles θ_{ij} and φ_{ij} introduced in the sites of the $M \times N$ regular lattice. The indices i and j, ($i = 1 \ldots M$, $j = 1 \ldots N$), determined the position along y and z axes, respectively. These discrete angles were used to express the free energy per unit area of the layer. Only the part which depends on the director orientation was taken into account. In the undistorted state this part was equal to zero. The stable states deformed by the electric field were due to negative energy. The final set of the angles and the spatial period due to equilibrium state were found in the course of an iteration process. The amplitudes A, B, D, F, G, H and the stripe width Λ were varied successively by small intervals, ΔA, ΔB, ΔD, ΔF etc. If the change led to the lower free energy then the changed variable was replaced by its new value and the interval was increased by a small factor. In the opposite case, the variable remained unchanged and the interval was decreased. This procedure was repeated until all the intervals became sufficiently small and further reduction in the free energy was negligible. Analogous method was successfully used in previous works concerning the homogeneous as well as periodic deformations of non-flexoelectric nematics [2,11–13].

If the layer parameters had suitable values, then the non-zero amplitudes A, B, G, and H as well as finite Λ were obtained, whereas D and F vanished, which denoted the appearance of periodic deformations. The results were quantitatively correct if the amplitudes were sufficiently low. Therefore, for each set of the layer parameters, the calculations were performed for a series of decreasing voltages. The threshold voltage U_0, was found as the voltage value determined by extrapolation of the amplitudes to zero. Simultaneously, the initial space period Λ_0 of the patterns was obtained. Such procedure was done for various sets of $\Delta\varepsilon$, Δe and k_{22}/k_{11}.

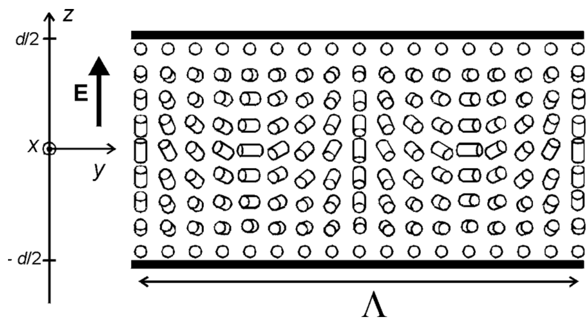

Figure 1. The structure of a single stripe illustrated schematically by means of cylinders symbolizing the director. The deviation of cylinders from the x direction is exaggerated.

4. Results

4.1. *Structure of the Stripes*

The computations showed that in the general case the structure of the patterns can be described by the formulae (1) and (2) in which $D = 0$ and $F = 0$. They represent the initial director distribution occurring just above the threshold. In the non-flexoelectric nematics, the periodic patterns arise only if $r < 0.3$, and create the PST stripes [2]. They are described by Eqs. (1) and (2) with $B = 0$ and $G = 0$. When the flexoelectric properties are very weak, the structure of the stripes is still similar to the PST case with dominating A and H. However, further increase of Δe leads to the structure, which is determined by dominating A and G amplitudes and differs from that due to the PST stripes. The structure of a single stripe of this type is illustrated schematically in Figure 1.

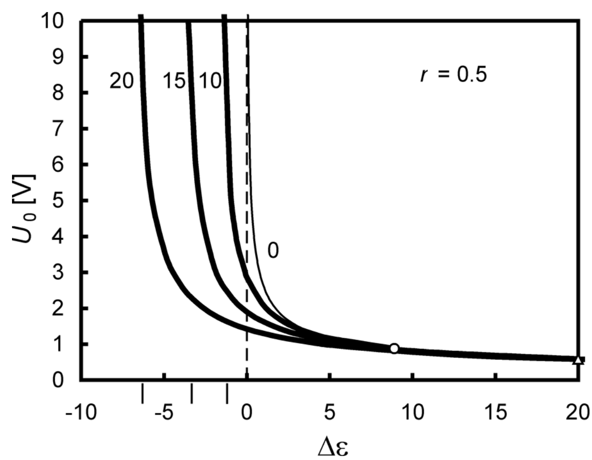

Figure 2. The threshold voltage for longitudinal domains U_0 as a function of dielectric anisotropy for three values of Δe (in pCm^{-1}) indicated at the curves; $r = 0.5$. The short lines below the horizontal axis denote the limiting values of dielectric anisotropy, $\Delta\varepsilon_1$. The circle and the triangle indicate the limiting values $\Delta\varepsilon_2$, for $\Delta e = 10$ and $15\,\mathrm{pCm}^{-1}$ respectively.

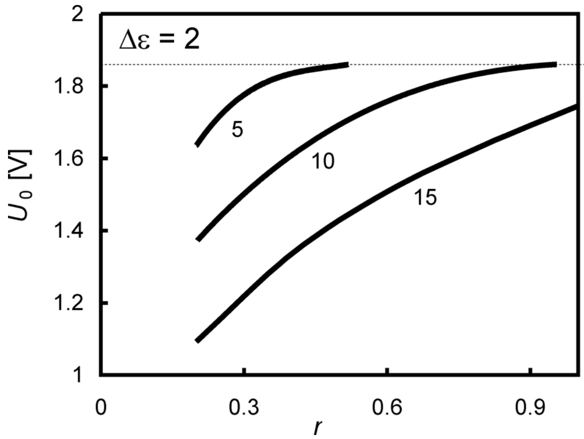

Figure 3. The threshold voltage for longitudinal domains U_0 as a function of elastic constants ratio $r = k_{22}/k_{11}$ for three values of Δe (in pCm^{-1}) indicated at the curves; $\Delta\varepsilon = 2$. Dashed line denotes the value of U_c.

4.2. *Threshold Voltage*

The longitudinal domains appear above certain threshold voltage, U_0, which is lower than the threshold $U_c = \pi[k_{11}/(\varepsilon_0\Delta\varepsilon)]^{1/2}$ for one-dimensional deformations. The threshold voltage for periodic deformations decreases with $\Delta\varepsilon$ and Δe but increases with r as it is shown in Figures 2 and 3. The domains arise above a limiting negative value of dielectric anisotropy $\Delta\varepsilon_1$ at which U_0 becomes infinite and below a positive value $\Delta\varepsilon_2$ at which the U_0 becomes equal to U_c (Fig. 2). When the dielectric anisotropy is higher than $\Delta\varepsilon_2$, then the one-dimensional deformations occur. In the non-flexoelectric nematic, the domains arise only if $r < 0.3$. However, if the nematic

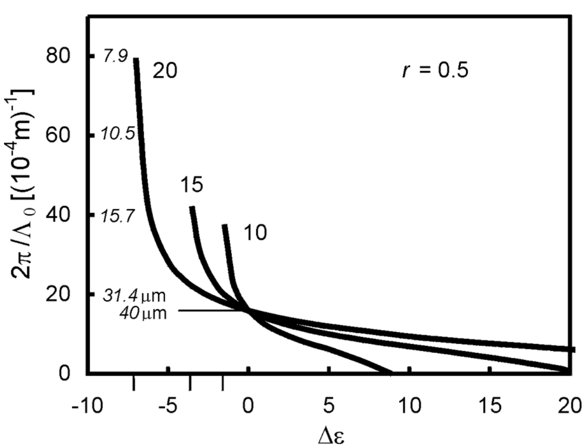

Figure 4. The initial wave number of longitudinal domains $2\pi/\Lambda_0$ as a function of dielectric anisotropy for three values of Δe (in pCm^{-1}) indicated at the curves; $r = 0.5$. The values of the spatial period Λ_0 (in micrometers) are also shown on the vertical scale. The short lines below the horizontal axis denote the limiting values of dielectric anisotropy, $\Delta\varepsilon_1$.

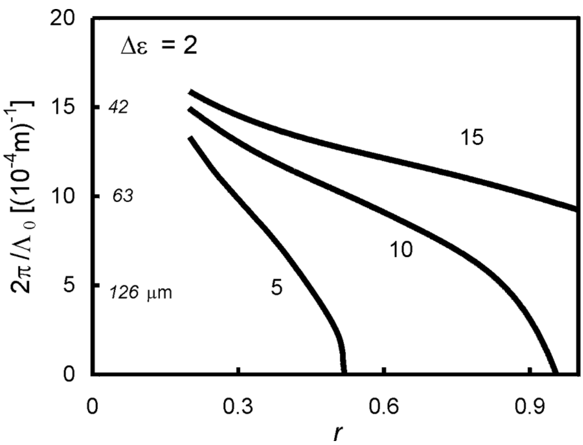

Figure 5. The initial wave number of longitudinal domains $2\pi/\Lambda_0$ as a function of elastic constants ratio $r = k_{22}/k_{11}$ for three values of Δe (in pCm^{-1}) indicated at the curves; $\Delta\varepsilon = 2$. The values of the spatial period Λ_0 (in micrometers) are also shown on the vertical scale.

possesses flexoelectric properties, this limiting upper value of the ratio r increases with Δe (Fig. 3). The deformations become one-dimensional at this limiting ratio.

4.3. *Wave Number or Spatial Period*

Typically, the domains arising at the threshold voltage have finite spatial period Λ_0. However Λ_0 becomes infinite when the dielectric anisotropy and the elastic constants ratio reach their upper limiting values. As a result, the domains disappear and are replaced by the one-dimensional deformation. These features are illustrated in Figures 4 and 5 by means of the wave number q. In the dielectrically compensated

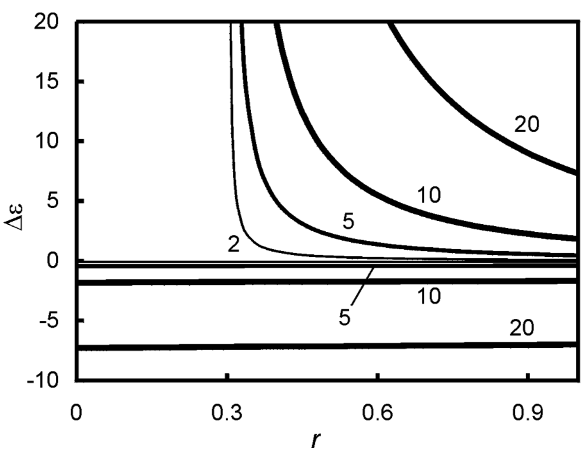

Figure 6. The regions of existence of the longitudinal domains in the parameter plane (r, $\Delta\varepsilon$). For given value of Δe indicated in pCm^{-1} at each pair of the curves, the domains exist if the parameters belong to the area between the curves.

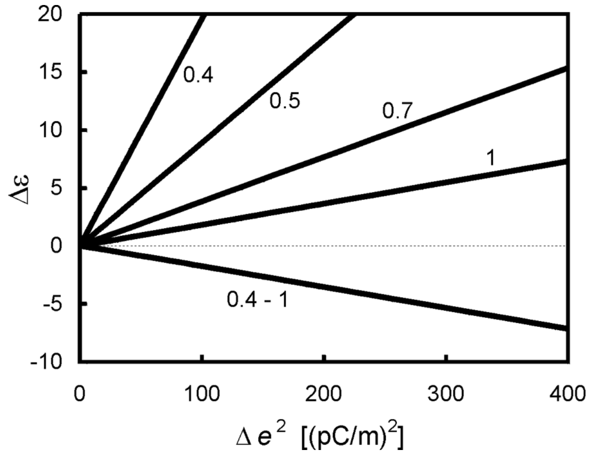

Figure 7. The regions of existence of the longitudinal domains in the parameter plane ($\Delta\varepsilon$, Δe^2). The values of r are indicated at each pair of the curves. (The lowest line denotes the lower boundaries which are practically independent of r.) For given value of r, the domains exist if the parameters belong to the area between the lines of each pair.

nematics, the spatial period Λ_0 is equal to double thickness of the layer. This peculiar property agrees with experiment [6] as well as with theoretical predictions [7].

4.4. *Regions of Existence of the Domains*

The longitudinal domains can arise in nematics characterised by both positive and negative dielectric anisotropy as it is shown in Figure 6. If $\Delta e = 0$, the domains exist for any positive value of $\Delta\varepsilon$ but only if $r < 0.3$. If $\Delta e \neq 0$, then the domains can appear for any r. The corresponding range of $\Delta\varepsilon$ includes both positive and negative

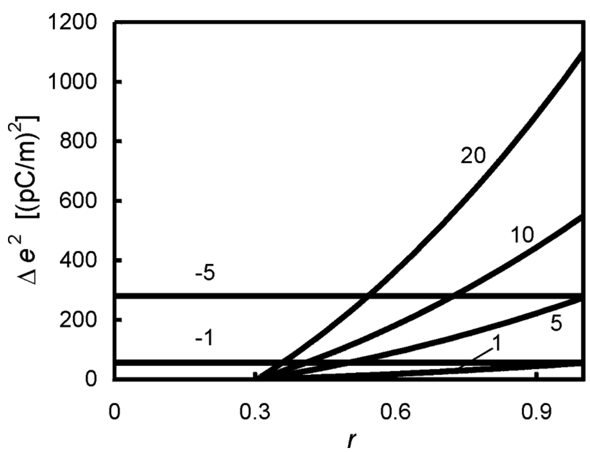

Figure 8. The regions of existence of the longitudinal domains in the parameter plane (r, Δe^2). For given value of $\Delta\varepsilon$ indicated at each curve, the domains exist if the parameters belong to the area above the curve.

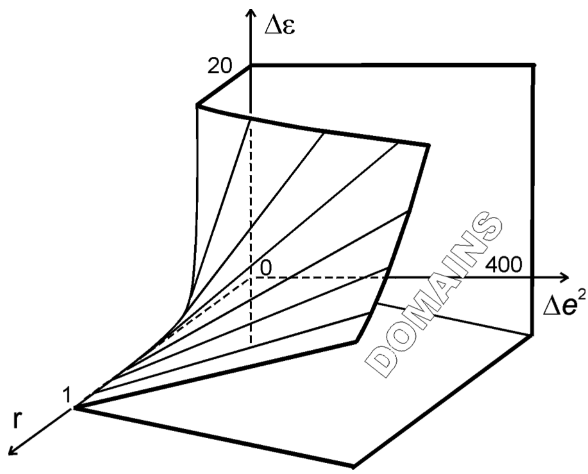

Figure 9. The surface in the parameter space (r, Δe^2, $\Delta\varepsilon$) which limits the region of existence of the domains. The quantity Δe^2 is expressed in $pC^2\,m^{-2}$.

values, however for low Δe and above $r = 0.3$ it is extremely narrow. It widens proportionally to Δe^2 as it is presented in Figure 7. Figure 8 shows that the higher the absolute value of dielectric anisotropy is, the larger must be the flexoelectric parameter above which the stripes can exist. Above statements are summarized in Figure 9 where the surface which limits the region of existence of the domains in the parameter space (r, Δe^2, $\Delta\varepsilon$) is shown.

5. Summary

The calculations confirmed that the influence of flexoelectric properties depends on the absolute value of the difference $e_{11} - e_{33}$. In general, flexoelectricity enhances the ranges of parameters for which the domains exist. It affects also the structure of the periodically deformed layer. The $U_0(\Delta\varepsilon)$ dependence agrees qualitatively with the experimental data presented in [6]. The ranges of the dielectric anisotropy, flexoelectric parameter and elastic constants ratio for which the patterns exist, were determined.

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