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D. Andrienko^a & Yu. Reznikov^a

^a Institute of Physics, 46 Prospect Nauki, Kyiv, Ukraine, 252650 E-mail:

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Orientational Transitions in a Nematic Cell with Reverse Director Distributions

D. ANDRIENKO, YU. REZNIKOV

Institute of Physics, 46 Prospect Nauki, Kyiv, Ukraine 252650,
denis@marion.iop.kiev.ua

We predict orientational transitions in a nematic cell with co-directed and reversed orientations of easy axes on the aligning surfaces. Aside from a *forward* director distribution there can exist the *reverse* distributions with zero and $\pi/2$ polar director angle at some point in the cell bulk. In the Rapini approach for the surface free energy these distributions can be unstable and transition two the forward distribution can occur. Dimensionless parameters, controlling the director distribution are the easy axis angle and an anchoring strength parameter WL/K .

Keywords: liquid crystal; orientational transitions

INTRODUCTION

Present-day possibility to control the liquid crystal (LC) alignment allows to investigate the non-uniform director distributions in searching for new astonishing effects and applications^[1]. Special attention is paid to the cells with possible orientational transitions of the director^[2–6]. In particular, reorientation of the director in a hybrid (homeoplanar) cell with mutually orthogonal easy axis directions on the opposite surfaces is studied carefully^[4–6]. Three types of the director distributions are possible in this geometry: 1) homeotropic, with director normal to plates; 2) planar, with director parallel to them; 3) tilted (hybrid), with non-uniform director orientation in the cell. The threshold reorientation between these distributions takes place under the variation of the anchoring strength on the cell surfaces. Character of

transitions between them depends on the anisotropy in Frank elastic constants and is the second-order in the one-elastic-constant approximation and the first-order for typical LCs with $K_1 = K_3 = 2K_2$.

Further consideration of flat director distributions in the cell with arbitrary easy axis directions on the aligning surfaces leads to some novel features. As it was noted, several distributions can minimize the cell free energy [7]. Among them the energetically lowest are so called forward (Fig. 1a), reverse-planar (Fig. 1b) and reverse-homeotropic (Fig. 1c) distributions.

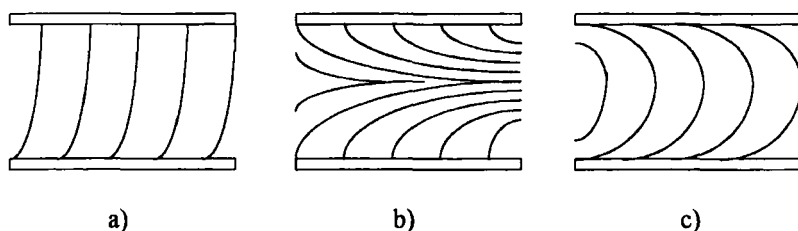


FIGURE 1. a) forward, b) planar reverse, c) homeotropic reverse director distributions

Simple comparison of their free energies shows that under the strong anchoring on the surfaces and in the one-elastic-constant approximation all distributions are stable and the forward distribution is the most energetically favorable. The homeotropic reverse distribution is preferable than the planar reverse distribution if the sum of the tilt angles on the bounding planes exceeds $\pi/2$, otherwise the planar reverse distribution is preferable. The forward distribution is the global minimum of the LC free energy. Homeotropic and planar reverse distributions minimize it locally.

The reverse distributions are quite useful for applications. First, they are bistable in the applied electric or magnetic field^[7-10]. Second, transitions between them have fast electro-optical response because of no "back flow" and are characterized by low power consumption^[11].

In our article we study stability of the reverse director distributions in polar plane. First, in Sec.1, we obtain general expressions for the free energies of the reverse distributions of the director in the polar plane. Then, in Sec.2,3, we study these distributions and their stability.

1. FREE ENERGY OF THE REVERSE DISTRIBUTIONS

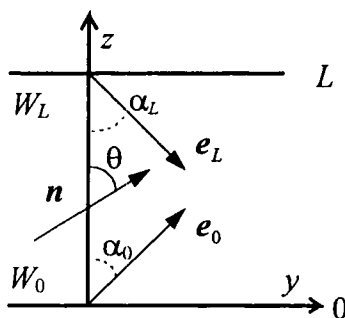
Let us formulate the problem we are dealing with in more detail. We consider

the nematic LC of thickness L bounded by the surfaces $z = 0, L$. The director \mathbf{n} is assumed to be parallel to the yz plane and to depend only on z coordinate. The surfaces are able to orient adjacent liquid crystal molecules and the degree of that anchoring is characterized by the surface free energy. To describe it, we use model expression, first proposed by Rapini and Papoular^[12] $F_{RP} = -\frac{1}{2}W \int (\mathbf{n}\mathbf{e})^2 dS$, where \mathbf{e} is a unit vector along the easy axis direction, W is an anchoring energy.

In the notations given there the orientational field may be written as $\mathbf{n} = (0, \cos\theta, \sin\theta)$, $\theta = \theta(z)$, which transforms the LC free energy^[13] into

$$F/S = \frac{1}{2} \int_0^L f_{13}(\theta) \dot{\theta}^2 dz + F_s, \quad (1)$$

where $f_{\alpha\beta}(\theta) = K_\alpha \sin^2 \theta + K_\beta \cos^2 \theta$, $\dot{\theta} = \frac{\partial \theta}{\partial z}$, K_i are Frank elastic constants, $F_s = -\frac{1}{2}W_0 \cos^2(\theta_0 - \alpha_0) - \frac{1}{2}W_L \cos^2(\theta_L - \alpha_L)$ is the surface free energy, $\theta_{0,L} = \theta(z=0, L)$ are director tilt angles,



are director tilt angles, $\mathbf{e}_{0,L} = (0, \sin \alpha_{0,L}, \mp \cos \alpha_{0,L})$ are the unit vectors along the easy axis directions, W_L, W_0 are the anchoring energies on the surfaces $z = 0, L$ correspondingly. Considered geometry is sketched in Fig.2.

The free energy density (1) does not depend explicitly on z ; thus it admits the first integral given by $\dot{\theta} \frac{\partial f}{\partial \dot{\theta}} - f = I$, where

FIGURE 2. Considered geometry

I is a constant. Thus, along with the boundary conditions, obtained from the minimization of the free energy (1), the boundary problem for the director angle takes the form

$$\begin{cases} f_{13}(\theta) \dot{\theta}^2 = I \\ 2f_{13}(\theta_{0,L}) \dot{\theta}|_{z=0,L} = \pm W_{0,L} \sin 2(\theta_{0,L} - \alpha_{0,L}) \end{cases} \quad (2)$$

The constant of integration I depends on the director tilt angles and can be

found from (2) as $I = \frac{1}{L} \int_{\theta_0}^{\theta_L} d\theta \sqrt{f_{13}(\theta)}$.

Performing an integration of the free energy (1) we obtain the free energies of the forward, homeotropic and planar reverse distributions of the director correspondingly

$$F_{ag}/F_0 = [E(\theta_L, \delta_1) - E(\theta_0, \delta_1)]^2 + f_s, \quad (3)$$

$$F_{rh}/F_0 = [E(\theta_L, \delta_1) + E(\theta_0, \delta_1)]^2 + f_s, \quad (4)$$

$$F_{rp}/F_0 = [2E(\frac{\pi}{2}, \delta_1) - E(\theta_L, \delta_1) - E(\theta_0, \delta_1)]^2 + f_s. \quad (5)$$

Here $F_0 = \frac{SK_3}{2L}$, $E(\theta, \delta) = \int_0^\theta dx \sqrt{1 - \delta \sin^2 x}$ is the incomplete elliptic integral

of the second kind, $f_s = -\xi_0 \cos^2(\theta_0 - \alpha_0) - \xi_L \cos^2(\theta_L - \alpha_L)$, $\delta_1 = (K_3 - K_1)/K_3$, $\xi_i = W_i L/K_3$. Integrating the expression for the free energy (1) we take into account that for the reverse-homeotropic distribution director angle changes within the range $[\theta_0, -\theta_L]$ and is equal to zero under some value of z coordinate, for the reverse planar it changes in the same range but through $\pi/2$, and for the forward distribution this range is $[\theta_0, \theta_L]$.

Minimizing the free energies (3)-(5) with respect to θ_0, θ_L we can obtain the equations for the tilt director angles. Before the minimization let us study the character of dependencies of expressions (3)-(5) on θ_0, θ_L i.e. the stability of corresponding director distributions.

Below we pay attention to the particular boundary conditions which lead to the threshold director reorientation and can be realized experimentally.

2. REVERSE-PLANAR DISTRIBUTION

Let one bounding surface possesses strong director anchoring, $\xi_L = \infty$, so that $\theta_L = \alpha_L$. Also we assume that the other surface provides homeotropic anchoring, i.e. $\alpha_0 = 0$. Hence, two parameters characterize the director distribution in the cell: the tilt angle α_L and the anchoring parameter ξ_0 .

Under such boundary conditions the dependence of the reverse-planar free energy (5) on the tilt angle θ_0 plotted for the different anchoring energies ξ_0 is typical for the first-order transition (Fig.3.a). The anchoring parameter ξ_0 plays the role of 'temperature' and the tilt angle θ_0 -- of 'order parameter'. Therefore, the director distribution has a jump-like behavior under the smooth variation of ξ_0 .

Thus, if the anchoring parameter ξ_0 reaches the threshold value $\xi^{th}(\alpha_L)$ the tilt angle θ_0 changes discontinuously from the value minimizing the planar reverse free energy to $\pi/2$. Further reorientation of director strongly depends on the morphology of the aligning surface. If the LC molecules near the aligning surface can rotate on the angle more than $\pi/2$ the reverse-planar distribution transits to the forward one. Since the forward distribution is stable under all changes of the anchoring parameter, the reversed transition is impossible. Another situation is also reasonable, when LC molecules (and the director) are limited in rotation by the $\pi/2$ angle. In this case the first-order transition (without hysteresis) will occur between reverse-planar distribution and distribution with tilt angle $\theta_0 = \pi/2$.

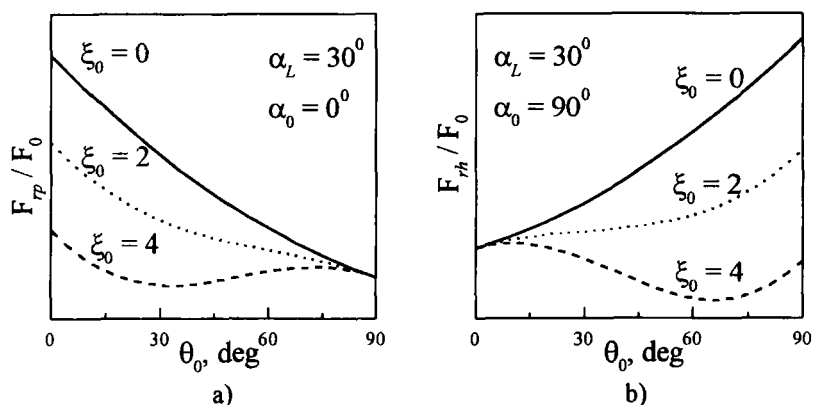


FIGURE 3. Typical for the first-order transitions free energy dependence on the tilt angle for the a) reverse-planar and b) reverse-homeotropic distributions.

Let's find the threshold anchoring ξ^{th} as the function of the tilt angle α_L . To do this note, that the director distribution in the cell gives the extremum of the total free energy (5), so that

$$\partial F_r / \partial \theta_0 = 0. \quad (6)$$

The solution to the equation (6) is stable only if $\partial^2 F_r / \partial \theta_0^2 > 0$. Thus, the equation $\partial^2 F_r / \partial \theta_0^2 = 0$ together with (6) defines the dependence $\xi^{th}(\alpha_L)$. Evaluation of derivatives gives this dependence in parametric form

$$\xi^{th} = - \frac{(1 - \delta_1 \sin^2 \theta_0)^2}{\cos 2\theta_0 + \delta_1 \sin^4 \theta_0}, \quad (7)$$

$$E(\alpha_L, \delta_1) = 2E\left(\frac{\pi}{2}, \delta_1\right) - E(\theta_0, \delta_1) + \frac{1}{2} \sin 2\theta_0 \frac{(1 - \delta_1 \sin^2 \theta_0)^{3/2}}{\cos 2\theta_0 + \delta_1 \sin^4 \theta_0},$$

where the tilt angle θ_0 , serves here as parameter. Calculated dependence $\xi^{th}(\alpha_L)$, is shown in Fig.4,a).

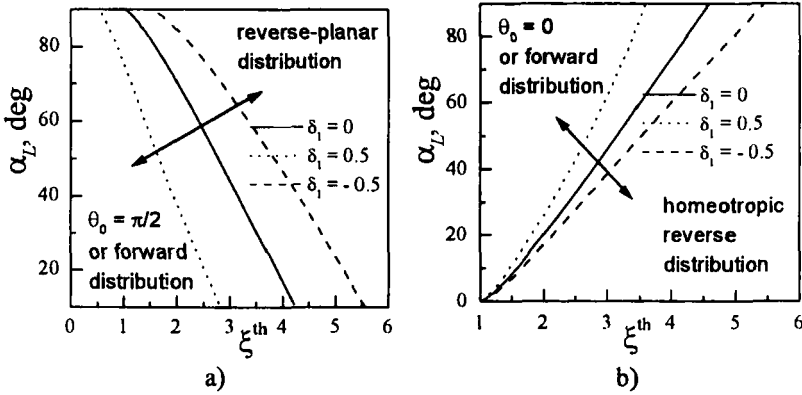


FIGURE 4. Transition line calculated for different values of anisotropy in Frank's elastic constants. a) for the transition from reverse-planar distribution; b) for the transition from reverse-homeotropic distribution

3. REVERSE-HOMEOTROPIC DISTRIBUTION

The free energy density $f(K_1, K_3, \theta, \alpha_0, \alpha_L)$ in Eq.(1) is invariant with respect to the substitution $(K_1, K_3, \theta, \alpha_0, \alpha_L) \rightarrow (K_3, K_1, \pi/2 - \theta, \pi/2 - \alpha_0, \pi/2 - \alpha_L)$. This substitution transform the planar reverse distribution to the homeotropic reverse one. Thus, the homeotropic reverse distribution, realized in the cell with one planar easy axis is absolutely similar in the description to the reverse planar distribution in the cell with one homeotropic easy axis. It is immediately obvious, that the homeotropic reverse distribution in the cell with $\xi_L = \infty$ and $\alpha_0 = \frac{\pi}{2}$ has the first-order transition to the distribution with $\theta_0 = 0$ (Fig.3,b). Further transition to the forward state is also possible and, moreover, there are no restrictions on the rotation of director. Threshold anchoring parameter as the function of the tilt angle can be obtained from Eq.(7) by substituting $\delta_1 \rightarrow \delta_1/(\delta_1 - 1)$, $\alpha_L \rightarrow \pi/2 - \alpha_L$ and is shown in Fig.4,b).

4. CONCLUSIONS

We consider orientational transitions in a nematic liquid crystal cell with co-directed easy axes on the aligning surfaces. Several distributions of the director can minimize the free energy of the cell with such boundary conditions. The most energetically favorable distributions are the planar and homeotropic reverse director distributions. Stability of these distributions depends on the anchoring of LC with the bounding planes and directions of the easy axes. In particular, the reverse-planar distribution realized in the cell with one easy axis of infinite strength and the other homeotropic easy axis with finite anchoring can be unstable. Transition from it to the distribution with the tilt angle $\frac{1}{2}\pi$ or to the forward distribution was found to be the first-order. In its turn, the reverse-homeotropic distribution also possesses analogous transition to the distribution with zero tilt angle (or forward distribution) in the cell with one rigid easy axis and one weak planar easy axis.

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