PIEZOELECTRIC DOMAINS IN LIQUID CRYSTALS

S. G. DMITRIEV

L. D. Landau Institute of Theoretical Physics, USSR Academy of Sciences

Submitted May 18, 1971

Zh. Eksp. Teor. Fiz. 61, 2049–2052 (November, 1971)

The possibility of formation of piezoelectric domains in nematic liquid crystals located in an electric field is considered. It is pointed out that domains are not produced in region (4) $\epsilon_\perp$ and $\epsilon_\parallel$ are respectively the nematic liquid crystal dielectric constants in the directions perpendicular and parallel to the molecular symmetry axis of the liquid crystal and k and e are the elastic and piezoelectric constants).

WE investigate in this paper the possibility of formation of piezoelectric domains in a nematic liquid crystal placed in an electric field. We show that the problem has a region of parameters in which no domains are produced.

1. Meyer[1] investigated the piezoelectric domains formed in the presence of an electric field in a nematic liquid crystal (NLQ). He established in his paper that a periodic structure (domains) with period Δ (see below) is produced in a piezoelectric NLQ under the influence of the field. In solving the problem, Meyer used the macroscopic theory developed in[2-4], according to which the energy of perturbation of a unit volume of the NLQ is, in the lowest order, a quadratic function of the gradients of $\mathbf{n}(\mathbf{r})$, and is given by the expression

$$H_b = {}^1/_2[k_{11}(\operatorname{div}\mathbf{n})^2 + k_{22}(\mathbf{n}\operatorname{rot}\mathbf{n})^2 + k_{33}[\mathbf{n}\operatorname{rot}\mathbf{n}]^2], \qquad (1)$$

where $\mathbf{n}$ is the unit vector describing the preferred direction of the molecule axes of the liquid crystal at the point $\mathbf{r}$. In the presence of an electric field the energy of the system contains, besides the self-energy of the field and the perturbation energy (1), also two piezoelectric terms: $4\pi e_1(\mathbf{E}\cdot\mathbf{n})\operatorname{div}\mathbf{n}$ and $4\pi e_2\mathbf{E}[(\mathbf{n}\cdot\nabla)\times\mathbf{n}]$ (see[1]), where $\mathbf{E}$ is the electric field intensity.

Meyer investigated the functional

$$\int\left(H - \frac{\mathbf{ED}}{4\pi}\right)dV,$$

where H is the total energy per unit volume and $\mathbf{D}$ the dielectric induction vector. We introduce the symbol

$$\tilde{H} = H - \mathbf{ED}/4\pi = {}^1/_2[k_{11}(\operatorname{div}\mathbf{n})^2 + k_{22}(\mathbf{n}\operatorname{rot}\mathbf{n})^2 + k_{33}[\mathbf{n}\operatorname{rot}\mathbf{n}]^2] - e_1(\mathbf{En})\operatorname{div}\mathbf{n} - e_2\mathbf{E}(\mathbf{n}\nabla)\mathbf{n} - \frac{1}{8\pi}[\varepsilon_\perp\mathbf{E}^2 + (\varepsilon_\parallel - \varepsilon_\perp)(\mathbf{nE})^2], \qquad (2)^*$$

where $\epsilon_\perp$ and $\epsilon_\parallel$ are the dielectric constants of the NRQ in the directions perpendicular and parallel to the symmetry axis of the liquid-crystal molecules, respectively. The last term in (2) corresponds to the self-energy of the field in the expressions for the energy.

The problem consists of minimizing the functional $\int\tilde{H}dV$ and solving Maxwell's equations. Meyer makes the following simplifying assumptions:

$$k_{11} = k_{33} = k, \quad e_1 = -e_2 = e, \quad \varepsilon_\parallel = \varepsilon_\perp, \quad E_y = E_0 = \text{const}, \quad E_x = 0$$

*$(\mathbf{n}\operatorname{rot}\mathbf{n})^2 \equiv (\mathbf{n}\cdot\operatorname{rot}\mathbf{n})^2$; $[\mathbf{n}\operatorname{rot}\mathbf{n}] \equiv \mathbf{n}\times\operatorname{rot}\mathbf{n}$.

and considers a planar model of the NLQ, namely

$$n_x = \cos\theta, \quad n_y = \sin\theta, \quad \theta = \theta(x), \qquad (3)$$

where θ is the angle between $\mathbf{n}(\mathbf{r})$ and the Ox axis. Then

$$H = \frac{1}{2}k\left(\frac{d\theta}{dx}\right)^2 + eE_0\left(\frac{d\theta}{dx}\right).$$

Minimizing this functional, Meyer obtains a periodic solution $\theta = eE_0x/k$ with period $\Delta = \pi k/eE_0$.

Thus we see that the electric field produces a domain structure with a period Δ. This structure vanishes with decreasing E_0, and the period tends at the same time to infinity. It turns out, however, that if $\alpha = \epsilon_\parallel - \epsilon_\perp \neq 0$, then domains are not produced at all values of e and k; it will be shown below that in the region where

$$|\alpha| - e^2\pi^3/k > 0, \qquad (4)$$

there is no domain structure and a homogeneous state is produced.

2. We consider a planar model of the NLQ, introduce the notation (3), and make the simplifying assumptions $k_{11} = k_{33} = k$, $e_1 = -e_2 = e$, but assume that $\alpha \neq 0$. As indicated above, the problem consists of investigating the "energy" $\int\tilde{H}dV$ and solving Maxwell's equations. Let us solve these equations: from curl $\mathbf{E} = 0$ we readily obtain $E_y \equiv E_0 = \text{const}$, $E_x = E(x)$; we consider further the equation div $\mathbf{D} = 0$, where (see[1])

$$\mathbf{D} = \varepsilon_\perp\mathbf{E} + \alpha\mathbf{n}(\mathbf{nE}) + 4\pi\{e_1\mathbf{n}\operatorname{div}\mathbf{n} + e_2(\mathbf{n}\nabla)\mathbf{n}\}$$

We put $D_x = 0$; then

$$\varepsilon_\perp E_x + \alpha E_x\cos^2\theta + \alpha E_0\cos\theta\sin\theta = 0; \qquad (5)$$

since usually $\alpha/\epsilon_\perp \ll 1$, we neglect terms of higher order in $\alpha/\epsilon_\perp$; it then follows from (5) that

$$E_x = -\alpha E_0\sin 2\theta/2\varepsilon_\perp.$$

With the same accuracy, we write down an expression for $\tilde{H}$:

$$\tilde{H} = \frac{1}{2}k\left(\frac{d\theta}{dx}\right)^2 + eE_0\frac{d\theta}{dx} - \frac{\varepsilon_\perp E_0^2}{8\pi}\left(1 + \frac{\alpha}{\varepsilon_\perp}\sin^2\theta\right). \qquad (6)$$

Minimizing $\tilde{H}$, we obtain

$$k\theta'' + \frac{\alpha E_0^2}{8\pi}\sin 2\theta = 0. \qquad (7)$$

We consider first the case when $\alpha > 0$. It follows from (7) that

$$\theta' = \pm\sqrt{A + \rho\cos 2\theta}, \quad \rho = \alpha E_0^2 / 8\pi k,$$

and A is the integration constant. We put $A \geq \rho$, and then the solution takes the form

$$px = \int_0^{\theta_0} \frac{d\theta}{\sqrt{1 - k_1^2 \sin^2\theta}} \quad p = \sqrt{A+\rho}, \quad k_1^2 = \frac{2\rho}{A+\rho} < 1 \qquad (8)$$

$$px = F(k_1, \theta_0)$$

(see[5]). The solution is periodic with a period

$$\frac{T}{4} = \int_0^{\pi/2} \frac{d\theta}{\sqrt{A + \rho - 2\rho\sin^2\theta}}. \qquad (9)$$

We note that as $A \to \rho$ the solution approaches the homogeneous one, and accordingly $T \to \infty$. We have to find the minimum "energy" per unit length for the domain structure, i.e., the minimum of the expression

$$I = \int \left[\frac{k}{2}(\theta')^2 + eE_0\theta' - \frac{\alpha E_0^2}{8\pi}\sin^2\theta\right]dx \Big/ \int dx$$

with respect to A (the integrals are taken over the period). Obviously, it is necessary to put sign $\theta' = -$ sign e, and then we obtain after trivial transformations

$$I_A' = \int_0^{\pi/2} (k\theta' - |e|E_0)\, d\theta \int_0^{\pi/2} \frac{d\theta}{2(\theta')^3} \Big/ \left(\int_0^{\pi/2} \frac{d\theta}{\theta'}\right)^2,$$

where $\theta' > 0$. Since $\int_0^{\pi/2} k\theta' d\theta$ is a monotonically increasing function of A at $A \geq \rho$, it is obvious that I will have a minimum at $A \geq \rho$ only if

$$\int_0^{\pi/2} (k\theta' - |e|E_0)\Big|_{A=\rho} d\theta < 0 \text{ or } \alpha - \frac{e^2}{k}\pi^3 < 0. \qquad (10)$$

If

$$\alpha - e^2\pi^3/k > 0 \qquad (11)$$

then the homogeneous state with $\theta_0 = \pi/2$ is more favored energywise (the value of θ_0 can be easily obtained from the expression (6) for $\widetilde{H}$).

Thus, if (10) holds true, a domain structure is produced and the solution is given in this case by expression (8), where k_1, and consequently also A, can be obtained from the expression

$$\int_0^{\pi/2} k\theta' d\theta = |e|E_0\frac{\pi}{2}, \quad \frac{E(k_1)}{k_1} = \frac{|e|E_0\pi}{2k\sqrt{2\rho}}, \qquad (12)$$

where $E(k_1)$ is a complete elliptic integral.

The case $\alpha < 0$ is perfectly analogous to the preceding case; its investigation leads to the general condition (4) for domain formation, but the homogeneous state arising when $A \to \rho$ will be somewhat different, namely $\theta_0 = 0$.

3. Let us consider some limiting situations. We note that if $\alpha = e^2\pi^3/k$ the solution can be obtained in terms of elementary functions. Indeed, from (12) we get $k_1 = 1$ and $A = \rho$, and then (8) takes the form

$$\sqrt{2\rho}\, x = \int_0^{\theta_0} \frac{d\theta}{\sqrt{1 - \sin^2\theta}} \text{ or } \sin\theta_0 = \operatorname{th}\sqrt{2\rho}\, x.$$

The period of the structure becomes infinite in this case. We see furthermore that as $\alpha \to 0$ the solution of (8) goes over into Meyer's solution (it is easy to obtain $\sqrt{A} = |e|E_0/k = \theta'$) from (12)) with a period Δ.

If the field is varied for a given substance, i.e., for a specified nonzero α, then, as seen from (12), k_1 remains unchanged, and A is proportional to ρ or $A \sim E_0^2$. Consequently $T \sim 1/\sqrt{\rho} \sim 1/E_0$ and we see that when the field is decreased, the period of the domain structure increases and tends to infinity, corresponding to a transition to the homogeneous state, and conversely, when the field increases, the period decreases and tends to zero. Formula (9) can then become incorrect if the period becomes of the same order as the microscopic distances characteristic of NLQ, since the chosen macroscopic approach no longer holds in this case.

We note finally that the investigation of the planar model of NLQ leads to the following result: the domain structure is produced when (10) is valid, and the solution in this case is periodic with a finite period (see (8) and (9)). The parameter A can be obtained from (12). On the other hand, if (11) is satisfied and there are no domains, then a homogeneous state with θ = const is formed ($\pi/2$ for $\alpha > 0$ and 0 for $\alpha < 0$). The results are valid in the region where the macroscopic theory is valid.

In conclusion, the author is sincerely grateful to I. E. Dzyaloshinskiĭ for suggesting the problem and for guiding the work.

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Translated by J. G. Adashko
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