A NEW TYPE OF DISCLINATION IN LIQUID CRYSTALS AND THE STABILITY OF DISCLINATIONS OF VARIOUS TYPES

S. I. ANISIMOV and I. E. DZYALOSHINSKIĬ

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

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In nematic liquid crystals, along with ordinary disclinations in which the director lies in a plane perpendicular to the line of the disclination, there may exist, in principle, disclinations with a "volume" structure. Which type actually occurs depends on the relation between the elastic moduli K_{11}, K_{22}, and K_{33} of the substance: when $K_{22} > \frac{1}{2}K_{11} + \frac{1}{2}K_{33}$ the "plane" disclination is stable, and when $K_{22} < \frac{1}{2}K_{11} + \frac{1}{2}K_{33}$ the "volume" disclination is stable. The stability of disclinations with various Frank indices n is studied. It is shown that when the moduli are almost equal only disclinations with $n = \pm 1$ are stable. A "plane" disclination with $n = 2$ is stable only under the conditions $K_{22} > 2K_{33}$ and $K_{33} < K_{11}$. For disclinations with high indices the "plane" structures are certainly stable when $K_{22} \gg K_{11}, K_{33}$, and the "volume" structures are stable when $K_{33} \gg K_{22}, K_{11}$.

1. INTRODUCTION

ONE form of violation of the uniformity of the structure of a nematic liquid crystal is by so-called "disclinations." A disclination is a singular line, analogous to a dislocation line in an ordinary crystal, close to which the direction of the mean orientation of the molecules (the direction of the director) changes sharply. A theory of disclinations was constructed by Oseen and Frank[1] for the case of equal elastic moduli K_{11}, K_{22}, K_{33} of the liquid crystal, and by one of the authors[2] for arbitrary K. However, only one of the possible types of structure of disclinations was considered, namely, it was assumed that the director always lies in a plane perpendicular to the disclination axis (we shall call such a type a "plane" disclination). In fact, however, the equations of the theory also have solutions in which the director does not lie in one plane ("volume" disclinations). The first to study disclinations differing in structure from the disclinations of Oseen and Frank was, apparently, de Gennes. In his theory of Grandjean terraces[3], he introduced disclinations with the director lying in a "vertical" plane, i.e., in a plane passing through the singular line. However, the plane structure of such disclinations is to some extent an accidental circumstance, and is connected with the equality, assumed in the work of de Gennes, of the moduli $K_{11} = K_{22} = K_{33}$. Below we shall show that, whereas the "plane horizontal" structure (i.e., the structure of the type considered in[1,2]) is an exact solution of the equilibrium equations for arbitrary K_{ii}, the "plane vertical" structure for unequal K becomes essentially three-dimensional.

Another aspect of the theory of disclinations not investigated until now is the question of their stability. It is immediately clear from the fact that the energy of a plane disclination is proportional to the square n^2 of its Frank index (cf.[1,2]) that all disclinations with indices $|n| \geq 2$ are at best metastable with respect to decay into a certain number of disclinations with $|n| = 1$. In practice, however, in many cases, disclinations with $|n| \geq 2$ are found to be unstable to small perturbations, i.e., the extremal points corresponding to them are saddle points on the energy surface.[1)] In particular, there are cases when any disclination with an even index can be converted in a continuous manner into the uniform state, with the energy of the structure decreasing monotonically to zero over the whole path. Analogously, any disclination with an odd index can be converted continuously into a disclination with $n = \pm 1$. The latter is stable with respect to transition to the uniform state, by virtue of the topological law of conservation of the "parity" of the index in a rotation about the singular line, with the condition $n \to \pm \mathbf{n}$. The situation remains the same when volume disclinations are included in the treatment. Here also, there are cases in which a plane disclination is a saddle point and can be converted into a volume disclination, and vice versa.

The investigation performed below shows that, for almost equal values of the moduli K_{ii}, only the "elementary" disclinations with $n = \pm 1$ are stable; the plane disclination is stable when

$$K_{22} > \tfrac{1}{2}(K_{11} + K_{33}), \quad (1)$$

and the volume disclination is stable when

$$K_{22} < \tfrac{1}{2}(K_{11} + K_{33}). \quad (2)$$

The plane disclination with $n = 2$ becomes stable only when

$$K_{22} > 2K_{33}, \quad K_{33} < K_{11}. \quad (3)$$

Finally, plane disclinations with high indices become stable when $K_{22} \gg K_{11}, K_{33}$. Analogously, volume disclinations with large n are certainly stable when $K_{33} \gg K_{11}, K_{22}$.

Below we consider separately the case when K_{11}, K_{22}, and K_{33} are close in magnitude and the case of arbitrary moduli.

2. THE CASE $K_{11} \approx K_{22} \approx K_{33}$

The general expression for the energy associated with nonuniformity in the orientation of the director $\mathbf{n}$[1],

1) We take the opportunity to express our thanks to Yu. A. Dreĭzin and A. M. Dykhne, who drew our attention to this situation.

$$F = {}^1/_2 \int dV\{K_{11}(\operatorname{div}\mathbf{n})^2 + K_{22}'(\mathbf{n}\operatorname{rot}\mathbf{n})^2 + K_{33}[\mathbf{n}\operatorname{rot}\mathbf{n}]^2\}, \tag{4*}$$

is simplified substantially in the case of equal moduli[2)]:

$$F = \frac{K}{2}\int dV\left\{\left(\frac{\partial\mathbf{n}}{\partial x}\right)^2 + \left(\frac{\partial\mathbf{n}}{\partial y}\right)^2 + \left(\frac{\partial\mathbf{n}}{\partial z}\right)^2\right\}, \tag{5}$$

where $K \equiv K_{11} = K_{22} = K_{33}$. A disclination (with the singular line coinciding with the z-axis) is a self-similar solution of the variational problem with the functionals (4) and (5); this solution depends only on x/y, or, which amounts to the same thing, on the azimuthal angle χ in the cylindrical system of coordinates $r\chi z$. Transforming to this system, we obtain from (5)

$$\frac{K}{2}\int\frac{dr}{r}dz\int_0^{2\pi}d\chi\left(\frac{d\mathbf{n}}{d\chi}\right)^2.$$

Hence, the free energy per unit length of the disclination is expressed in the form

$$f = \frac{K}{2}\ln\frac{R}{a}\int_0^{2\pi}d\chi\left(\frac{d\mathbf{n}}{d\chi}\right)^2, \tag{6}$$

where, as always (cf.[1,2]), the logarithmic integral over r has been cut off on the large-distance side at a length R equal in order of magnitude to either the distance between neighboring disclinations or the dimensions of the vessel, and on the short-distance side at the interatomic distance a.

The extrema of the functional (6) can be found rapidly from a mechanical analogy: f coincides with the integral of the kinetic energy (χ is the time) of a point with mass $K\ln(R/r)$ moving over a sphere of unit radius. The trajectories in this case are great-circle circumferences, and the period of the motion is determined by the uniqueness condition[1,2]; $\mathbf{n}(2\pi) = \pm\mathbf{n}(0)$. Thus, in the case of equal-moduli, the disclination is established in such a way that the director **n** can rotate in any plane passing through the coordinate origin. If this plane coincides with the equatorial plane, we have an ordinary "plane horizontal" disclination[1,2]; if it coincides with one of the meridional planes, we have the above-mentioned "plane vertical" disclination of de Gennes[3]. If we introduce the coordinate system $\xi\eta\zeta$ with the ζ-axis perpendicular to the plane in which the director lies, the periodicity condition gives the usual formulas[1]:

$$n_\xi = \cos\frac{n\chi}{2}, \quad n_\eta = \sin\frac{n\chi}{2}, \quad n_\zeta = 0, \qquad f = \frac{\pi n^2}{4}K\ln\frac{R}{a}, \tag{7}$$

where the integer n is the Frank index.

We now proceed to investigate the stability of the solutions (7). We note first of all that the mechanical analogy cannot be used in studying the stability; inasmuch as, in mechanics, only the extremal points have physical meaning, whereas in the theory of liquid crystals any field of directions $\mathbf{n}(\chi)$ satisfying the periodicity condition retains a physical meaning. The extremal states are distinguished only by the fact that, in principal, they can be stationary. Actually, of the extremal points (7), only those states which correspond to an absolute (and, correspondingly, local) minimum of the functional (6) are stationary stable (or metastable) states of the functional (6). The extremal points corresponding to maxima or saddle points of (6) are non-stationary and should go over, after a short time, into states with lower energy. Therefore, to solve the problem of the stability of the solution (7) we must consider an arbitrary vector field n of the form

$$-\pi/2 \leqslant \theta \leqslant \pi/2 \tag{8}$$

and determine the sign of a functional that is quadratic, near the extremal point (7), in the small declinations θ and $\varphi_1 = \varphi - n\chi/2$.

Substitution of (8) into (6) gives

$$f = \frac{1}{2}K\ln\frac{R}{a}\int_0^{2\pi}(\theta'^2 + \cos^2\theta\varphi'^2)\,d\chi \tag{9}$$

or, to within squares of the declinations from the extremal point,

$$f_2 = {}^1/_2\int_0^{2\pi}d\chi(\theta'^2 - \varphi_0'^2\theta^2 + \varphi_1'^2). \tag{10}$$

For brevity, we have omitted the constant factor $K\ln(R/a)$ and, here and in the following, we denote derivatives with respect to χ by a prime; according to (7), $\varphi_0 = n\chi/2$. The functions θ and φ_1 must satisfy the periodicity condition:

$$\varphi_1(\chi + 2\pi) = \varphi_1(\chi), \quad \theta(\chi + 2\pi) = (-1)^n\theta(\chi). \tag{11}$$

The variations of the functional (9) associated with change of φ are always positive, and it is therefore sufficient to treat changes of the variation θ only, for which

$$f_2 = \frac{1}{2}\int_0^{2\pi}d\chi\left(\theta'^2 - \frac{n^2}{4}\theta^2\right). \tag{12}$$

It can be seen immediately, that for even n, when, according to (11), θ is a periodic function of χ, the functional (12) does not have a well defined sign. In particular, it is negative for any variation θ that does not depend on the angle χ. This circumstance is directly connected with the fact that, as one can easily convince oneself, for even n, the conical field of directions

$$n_\xi = \cos\vartheta_0\cos\frac{n\chi}{2}, \quad n_\eta = \cos\vartheta_0\sin\frac{n\chi}{2}, \quad n_\zeta = \sin\vartheta_0$$

with constant ϑ_0, is not extremal but has a lower energy than the extremal plane solution (7). Moreover, since the energy of the field with constant ϑ_0 is proportional to $\cos^2\vartheta_0$, there exists a continuous transition, with monotonically decreasing energy, from any disclination with an even index ($\vartheta_0 = 0$) to the uniform state ($\vartheta_0 = \pi/2$).

In the case of odd n, it is necessary to investigate the functional (12) in more detail. We shall make use of a standard method and expand the integrand in (12) in eigenfunctions $\theta_\lambda(\chi)$ of the Euler operator:

$$\frac{d}{d\chi}\frac{\partial L}{\partial\theta'} - \frac{\partial L}{\partial\theta} = -\lambda\theta, \quad L \equiv \frac{1}{2}\left(\theta'^2 - \frac{1}{4}\bar{n}^2\theta^2\right). \tag{13}$$

Then

$$\int d\chi\, L(\theta, \theta') = {}^1/_2\sum_\lambda \lambda\int d\chi\,\theta_\lambda^2,$$

and the positive-definiteness of the functional coincides

*$[\mathbf{n}\operatorname{rot}\mathbf{n}] \equiv \mathbf{n}\times\operatorname{curl}\mathbf{n}$.

2)To avoid misunderstandings, we note that the integrand in (5) differs from that in (4) by a total derivative.

with the condition that the eigenvalues of (13) be positive, In our case, Eq. (13) is the one-dimensional Schrödinger equation

$$\theta'' + (\lambda + {}^1/_4 n^2)\theta = 0 \qquad (14)$$

with the periodicity conditions (11). The eigenfunctions and eigenvalues have the form

$$\theta_\lambda = A \sin\frac{m\chi}{2}, \quad \lambda = \frac{m^2 - n^2}{4}, \qquad (15)$$

where, if n is even, m runs over all the even values ($m = 0, \pm 2, \pm 4, \ldots$), and if n is odd, m runs over the odd values ($m = \pm 1, \pm 3, \ldots$). It can be seen that only when $n = \pm 1$ are all the eigenvalues λ_m non-negative.

Thus, for equal moduli K_{11}, only the "elementary" disclinations with $n = \pm 1$ have been found to be stable. These disclinations are also stable under more general "non-self-similar" perturbations $\theta(r, \chi, z)$ (see Appendix 1). It is interesting to note that the instability of disclinations with other n to non-self-similar perturbations corresponds, in the terminology of the eigenvalue problem of the type (14), to the quantum-mechanical collapse of a particle to the center.

An interesting manifestation of the instability of a disclination with n = 2 is the non-singular solution, found by Cladis and Kleman,[4] of the problem of the structure of a liquid crystal poured into a long cylindrical vessel[3]). If the surface of the vessel is prepared in such a way that the director must be tangential to the surface or perpendicular to it (Fig. 1), the obvious solution of the problem is the "plane" disclination with n = 2. However, the tendency of the director to leave the plane of the disclination and become parallel to the axis of the cylinder, which makes the disclination unstable, also leads to the result that there exists a non-singular solution of the problem, which now, of course, ceases to be "self-similar". Choosing the axes $\xi\eta\zeta$ in (8) to be along the coordinate axes xyz, we write (5) in the form

$$F = {}^1/_2 \int dV\, \{(\nabla\theta)^2 + \cos^2\theta(\nabla\varphi)^2\}. \qquad (16)$$

The corresponding Euler equations have the form

$$\Delta\theta + \sin\theta\cos\theta(\nabla\varphi)^2 = 0,$$
$$\Delta\varphi - 2(\nabla\theta\nabla\varphi)\,\mathrm{tg}\,\theta = 0.$$

If we assume that φ depends only on χ, and θ only on r, the second equation goes over into $\varphi'' = 0$. The boundary conditions on the surface of the cylinder ($r = R$) give $\theta(R) = 0$ and $\varphi(R) = \chi$. Therefore, $\varphi = \chi + \text{const}$ is a solution of the problem, and for $\theta(r)$ we have the equation

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\theta}{dr}\right) + \sin\theta\cos\theta = 0.$$

Investigation (cf.[4]) shows that this equation has

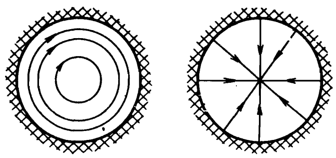

FIG. 1

[3])We are grateful to Dr. Kleman for sending a preprint of this work.

solutions satisfying the conditions $\theta(R) = 0$, $\theta(0) = \pi/2$, i.e., close to the axis of an unstable disclination with n = 2, the director is indeed parallel to the z-axis. One can also convince oneself that the energy of such a state is completely independent of the radius R of the vessel, i.e., it is much lower than the energy given by formula (7) for a disclination with n = 2.

Returning to disclinations with $n = \pm 1$, we note first of all that their stability when $K_{11} = K_{22} = K_{33}$ is neutral, inasmuch as the corresponding minimum eigenvalue, according to (15), is equal to zero. Actually, therefore, the stability criterion is now sensitive to small differences between the molecules. It is possible, in principle, to investigate the stability by the same general method when

$$\alpha = K_{33}/K_{11} - 1, \quad \beta = K_{22}/K_{11} - 1$$

are not equal to zero, by investigating the signs of the eigenvalues of the corresponding Euler operator. However, to determine the stability criterion in the approximation linear in the small parameters α and β, we can make use of simpler considerations (the equivalence of the two approaches is proved in Appendix 2).

We recall, first of all, that when $\alpha = \beta = 0$ the energy of the disclination does not depend on the orientation of the plane in which the director lies. The degeneracy is lifted, however, for non-zero α and β. We shall calculate the disclination energy as a function of the angle of inclination θ^* of its plane to the equatorial plane. In the zeroth approximation in α and β, the solution in the system $\xi\eta\zeta$ associated with the plane of the director has the form of (7) with $n = \pm 1$. For our calculations, the director in the "stationary" coordinate system xyz is also conveniently represented in the form of (8):

$$n_x = \cos\theta\cos\varphi, \quad n_y = \cos\theta\sin\varphi, \quad n_z = \sin\theta. \qquad (17)$$

Then, in the zeroth approximation in α and β, we have for the angles θ and φ

$$\sin\theta_0 = \sin\theta^*\sin(n\chi/2), \quad \mathrm{tg}\,\varphi_0 = \cos\theta^*\,\mathrm{tg}\,(n\chi/2). \qquad (18)$$

The energy of the disclination is now equal to the sum of the expression (9) and an expression linear in α and β:

$${}^1/_2 \int_0^{2\pi} d\chi\, \{\alpha(\theta'^2 + \cos^2\theta\varphi'^2)\cos^2\theta\sin^2\psi + \beta(\theta'\cos\psi + \varphi'\sin\psi\sin\theta\cos\theta)^2\}, \qquad (19)$$

where $\psi = \varphi - \chi$ is the azimuthal angle of the director in the natural system of coordinates (see Fig. 2). Since the solution (18) is itself an extremal point of the energy (9) for equal moduli, the required linear correction to the energy is given by the integral (19) with the unperturbed angles θ_0 and φ_0 (18). This gives

$$\Delta f/f = {}^1/_2\alpha(1 + \cos^2\theta^*) + \beta\sin^2\theta^* \qquad (20)$$

for both values $n = \pm 1$. (Here f is the unperturbed energy (9), $f = \pi/4$.)

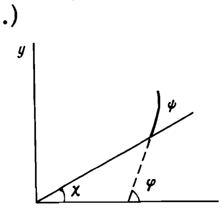

FIG. 2

It can be seen from formula (20) that the correction Δf to the energy is a monotonic function of the angle θ^* for values $0 < \theta^* < \pi/2$. At the points $\theta^* = \pi/2$ and $\theta^* = 0$, the correction takes the extremal values, equal to α and $\alpha/2 + \beta$ respectively. Therefore, for $\beta > \alpha/2$, which coincides with the condition (1), the "plane horizontal" disclination is stable and all the others are absolutely unstable. In the opposite case, $\beta < \alpha/2$ (the criterion (2)), only the "plane vertical" disclination is found to be stable.

In the region of its stability, in the same linear approximation in α and β, the "vertical" disclination ceases to be plane and acquires the "volume" structure mentioned in the Introduction. To determine it, it is necessary to solve the corresponding variational problem. We shall assume that, in the zeroth approximation in α and β, the director lies in the yz-plane, and describe the field n by the formulas (8) with $\zeta = x$, $\xi = y$ and $\eta = z$:

$$n_x = \sin\theta, \quad n_y = \cos\theta\cos\varphi, \quad n_z = \cos\theta\sin\varphi. \tag{21}$$

In the zeroth approximation, $\varphi_0 = n\chi/2$ and $\theta_0 = 0$. According to (4) and (21), the energy of the system can be written in the form of a sum of the expression (9) and the functional

$$\begin{aligned}{}^1/_2 \int_0^{2\pi} d\chi \, \{&\gamma[\theta'(\cos\theta\sin\chi + \sin\theta\cos\varphi\cos\chi) + \varphi'\cos\theta\sin\varphi\cos\chi]^2 \\ &+ \delta[\theta'\sin\varphi\cos\chi - \varphi'\cos\theta(\cos\theta\sin\chi + \sin\theta\cos\varphi\cos\chi)]^2\},\end{aligned} \tag{22}$$

where, in place of the constants α and β, we have introduced the quantities

$$\gamma = K_{11}/K_{33} - 1, \quad \delta = K_{22}/K_{33} - 1.$$

which are more convenient in our case.

We shall seek corrections θ and φ_1 that are linear in γ and δ and satisfy the boundary conditions (11) (with $n = \pm 1$). The corresponding equations have the form

$$\begin{gathered} n\varphi_1'' + \frac{5\gamma}{32}\sin\chi + \frac{2\delta - \gamma}{4}\sin 2\chi + \frac{5\gamma}{32}\sin 3\chi = 0, \\ \theta'' + \frac{1}{4}\theta = \frac{3\gamma - 2\delta}{16}\sin\frac{3\chi}{2} + \frac{6\delta - 5\gamma}{16}\sin\frac{5\chi}{2}. \end{gathered} \tag{23}$$

The periodic solution of the equation for φ_1 is given by the formula ($n = \pm 1$)

$$n\varphi_1 = \frac{5\gamma}{32}\sin\chi + \frac{2\delta - \gamma}{16}\sin 2\chi + \frac{5\gamma}{288}\sin 3\chi. \tag{24}$$

The solution of the equation for θ that satisfies the condition $\theta(2\pi) = -\theta(0)$ is not uniquely determined in the approximation linear in γ and δ. To the solution $\sim\sin(3\chi/2)$, $\sim\sin(5\chi/2)$ of the inhomogeneous equation, we can add a solution of the homogeneous equation, of the form[4)] $\sin(\chi/2)$. As always in problems of this type, the coefficient of $\sin(\chi/2)$ can be determined only in the next approximation in γ and δ, from the requirement that resonance terms $\sim\sin(\chi/2)$ cancel in the equation for θ_2. The corresponding calculations are trivial but very cumbersome, and so we give only their result:

$$\theta(\chi) = \frac{\delta^2 - \gamma\delta - {}^{29}/_{36}\gamma^2}{8(2\delta - \gamma)}\sin\frac{\chi}{2} + \frac{2\delta - 3\gamma}{32}\sin\frac{3\chi}{2} + \frac{5\gamma - 6\delta}{96}\sin\frac{5\chi}{2} \tag{25}$$

The first term in (25), proportional to $\sin(\chi/2)$, corresponds, as is easily seen, to a rotation of the plane of the disclination through a certain angle from its initial "vertical" position $\theta = 0$. The presence in addition to this term of two higher harmonics makes the structure of the disclination essentially non-planar. Thus, a "plane vertical" disclination exists only in the degenerate case when the elastic moduli are equal.

The first term in (25), describing the rotation of the plane, has a singularity when $\gamma = 2\delta$ or, in another form, when we have the relation $K_{22} = \frac{1}{2}(K_{11} + K_{33})$ between the elastic moduli. According to what was stated above, this equality corresponds (for almost equal moduli) to a stability change; in the zeroth approximation in γ and δ, the change in the structure consists of the rotation of the plane of the disclination through an angle $\pi/2$. Close to $\gamma = 2\delta$, the angle of rotation also remains finite in the first approximation, i.e., that with which the observed singularity is associated. We shall not refine the formula (25) close to $\gamma = 2\delta$ here, since this problem is only of academic interest.

3. DISCLINATIONS FOR ARBITRARY K_{11}, K_{22}, AND K_{33}

It has been established above that, for almost equal K_{11}, K_{22}, and K_{33}, all disclinations with Frank indices not equal to ± 1 are unstable. They become stable to small perturbations only when there are sufficiently large differences between the moduli. We begin by investigating plane disclinations. Following the standard method, we must find the eigenvalues of the Euler operator; the sign of these determines the stability. Since the exact solutions for a plane disclination with arbitrary K_{11}, K_{22}, and K_{33} are known[2], the problem can be solved, in principle, for each n. In practice, however, the exact solutions are so complicated that it is possible to obtain an answer in analytic form only for $n = 2$. In this case (cf.[2]), there exist two exact solutions: the first solution corresponds to the director lying along concentric circles, and the second to the director lying along radii passing through the disclination line (see Fig. 1). Using the formulas (9) and (19), we write the expression for the second variation of the energy:

$$f_{2\mathrm{I}} = \frac{1}{2K_{11}}\int_0^{2\pi} d\chi \, \{K_{33}\varphi_1'^2 + (K_{11} - K_{33})\varphi_1^2 + (K_{22} - 2K_{33})\theta^2 + K_{33}\theta'^2\}.$$

$$f_{2\mathrm{II}} = \frac{1}{2K_{11}}\int_0^{2\pi} d\chi \, \{K_{11}\varphi_1'^2 + (K_{33} - K_{11})\varphi_1^2 + K_{22}\theta'^2 - K_{11}\theta^2\}, \tag{26}$$

where $\varphi_1 = \varphi - \varphi_{\mathrm{I,II}}$ for the cases I and II respectively. It follows immediately from (26) (the boundary conditions for $n = 2$ permit constant φ_1 and θ) that the radial alignment of the director is always unstable and the alignment along the circles is stable for $K_{22} > 2K_{33}$, $K_{11} > K_{33}$ (criterion (3)).

Disclinations with large indices become stable for yet larger K_{22}, and as $K_{22} \to \infty$ all the plane disclinations become stable. The simplest way to convince oneself of this is by writing the expression proportional

4)The addition of the solution of the homogeneous equation that is proportional to $\cos(\chi/2)$ gives only a rotation of the plane of the disclination about the z-axis, as can be seen from (21), and can therefore be eliminated by a rotation of the coordinate system.

to $K_{22}(n \cdot \text{curl } n)^2$ in the natural components n_r, n_χ and n_z of the cylindrical coordinate system:

$$\frac{K_{22}}{2}\int_0^{2\pi} d\chi [n_r n_z' + n_z(n_\chi - n_r')]^2. \quad (27)$$

A plane disclination ($n_z = 0$) is an extremal point of the positive functional (27), making the latter vanish. Therefore, for very large $K_{22} \to \infty$, the plane disclination corresponds to the lowest energy value and, consequently, is stable.

The situation with the volume disclinations is more difficult, since we are unable to solve the variational problem for arbitrary K_{11}, K_{22}, and K_{33}. A general solution can be found only in the limit $K_{33} \to \infty$. The corresponding energy $K_{33}(n \times \text{curl } n)^2$ in the natural components is proportional to the integral

$$\frac{K_{33}}{2}\int_0^{2\pi} d\chi\, n_\chi^2 [(n_\chi - n_r')^2 + (n_\chi' + n_r)^2 + n_z'^2]. \quad (28)$$

The positive functional (28) has an extremum at $n_\chi = 0$, at which it vanishes. Therefore, by analogy with the case of a plane disclination in the limit $K_{22} \to \infty$, for large K_{33} volume disclinations with any index n for which $n_\chi = 0$ are stable. In such disclinations $n_r(\chi)$ and $n_z(\chi)$ are constant in each "vertical" half-plane χ = const. The corresponding "current lines" (tangential to the field n)

$$\frac{dr}{n_r} = \frac{d\chi}{0} = \frac{dz}{n_z}$$

are a family of parallel straight lines, lying in the "vertical" planes. The angle of inclination n_z/n_r depends on χ, i.e., varies from plane to plane (Fig. 3).

To determine the dependences $n_r(\chi)$ and $n_z(\chi)$, it is necessary to take into account the energy of the disclination in the next approximation, i.e., the functional (27) and the expression proportional to $K_{11}(\text{div } n)^2$:

$$\tfrac{1}{2}K_{11}\int_0^{2\pi} d\chi (n_r + n_\chi')^2. \quad (29)$$

Substituting

$$n_r = \cos\mu, \quad n_\chi = 0, \quad n_z = \sin\mu,$$

into the functional given by the sum of (27) and (29), we obtain

$$\tfrac{1}{2}\int_0^{2\pi} d\chi \{K_{22}\mu'^2 + K_{11}\cos^2\mu\}. \quad (30)$$

Since (30) does not contain χ explicitly, there exists the "energy" integral:

$$\tfrac{1}{2}K_{22}\mu'^2 + \tfrac{1}{2}K_{11}\sin^2\mu = C.$$

Hence it follows that χ can be expressed in terms of μ by means of an elliptic integral of the first kind:

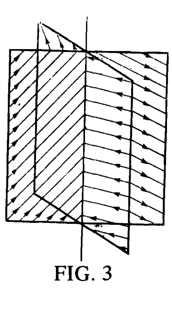

FIG. 3

$$\chi = \pm\varkappa\left(\frac{K_{22}}{K_{11}}\right)^{1/2}\int_0^\mu \frac{d\nu}{(1-\varkappa^2\sin^2\nu)^{1/2}}, \quad (31)$$

where in place of C we have introduced the new constant $\kappa^2 = K_{11}/2CK_{22}$. Correspondingly, the dependences on χ of the projections n_r and n_z of the director are given by the elliptic cosine and sine:

$$n_r = \text{cn}\left(\frac{\chi}{\varkappa}\sqrt{\frac{K_{11}}{K_{22}}}\right), \qquad n_z = \text{sn}\left(\frac{\chi}{\varkappa}\sqrt{\frac{K_{11}}{K_{22}}}\right). \quad (32)$$

The periodicity condition $\mu(2\pi) = \mu(0) + n\pi$ leads to the following formula connecting κ with n:

$$\pi = \varkappa|n|(K_{22}/K_{11})^{1/2}K(\varkappa), \quad (33)$$

where $K(\kappa)$ is a complete elliptic integral of the first kind.

The formulas (31)–(33) give a complete solution of the problem for any n. However, in view of the fact that they correspond only to the limiting case $K_{33} \gg K_{11}, K_{22}$, we shall not give a detailed study of them here.

4. CONCLUSION

We have seen above that, depending on the relations between the moduli K, two different types of disclination are possible: plane[1,2] and volume disclinations. The literature is comparatively poor in experimental data on the magnitudes of the elastic constants of nematic liquid crystals. Therefore, it does not appear possible to reach a more general conclusion on which type of disclination is the most common on the basis of these data. In those cases for which there are reliable data, the elastic moduli satisfy the inequalities $K_{33} > K_{11} > K_{22}$. For example, for p-azoxy-anisole[5,6], $K_{33} : K_{11} : K_{22} = 2.1 : 1 : 0.7$, and for p-n-methoxybenzylidine-p-butylaniline (MBBA)[6,7] these ratios are 1.1 : 1 : 0.5. Thus, only volume disclinations can exist in these substances.

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APPENDIX 1

Stability of Disclinations Under Non-self-similar Perturbations

In the general case, the stability is determined by the quadratic expansion of the functional (16):

$$f_2 = \frac{1}{2}\int dV\left\{(\nabla\varphi_1)^2 + (\nabla\theta)^2 - \frac{n^2}{4r^2}\theta^2\right\}.$$

In place of $(\nabla\varphi_0)^2$, for $\varphi_0 = n\chi/2$ we have substituted its expression in cylindrical coordinates, $n^2/4r^2$. As for self-similar perturbations also, the changes of f_2 for the variation φ_1 are positive. The Schrödinger equation analogous to (14) and corresponding to the Euler operator for f_2 has the form

$$\Delta\theta + (\lambda + n^2/4r^2)\theta = 0.$$

Its solution satisfying the periodicity conditions (11) has the form

$$\theta = R(r)e^{im\chi/2}e^{ikz},$$

where the parity of m is the same as the parity of n.

For R, we have the equation

$$-\frac{1}{r}\frac{d}{dr}\left(r\frac{dR}{dr}\right)+\left(\lambda-k^2+\frac{n^2-m^2}{4r^2}\right)R=0$$

and, for $n = \pm 1$, the function $R(r)$ has the form

$$R(r)=J_s(\varkappa r),\quad s^2=m^2-1,\quad m=\pm 1, \pm 3, \ldots,$$

where J_s is a Bessel function. In this case, $\lambda = \kappa^2 + k^2$, and the stability of the disclination is conserved. For other n there exist also, along with solutions of the same type as for $n = \pm 1$, solutions of the form

$$R(r)=K_{\pm i\sigma}(\varkappa r),\quad \sigma^2=n^2-m^2>0,$$

where $K_{i\sigma}$ is a Macdonald function. These solutions correspond in quantum mechanics to the collapse of a particle to the center. As is well known (cf., e.g.,[8]), in this case there exist arbitrarily low energy levels λ.

APPENDIX 2

The equivalence of the standard and energy approaches used in this paper is based on the fact that the "dangerous" perturbation giving the zero eigenvalue and having, according to (15), the form $\theta = \theta^* \sin(n\chi/2)$ gives, principally, only a rotation of the $\xi\eta$-plane (see formula (8)) in which the director rotated for $\alpha = \beta = 0$, through a small angle θ^*, i.e., the "dangerous" perturbation basically describes the transition from one of the solutions of the type (17), (18) to the other. Since, according to (20), all disclinations apart from "plane horizontal" and "plane vertical" disclinations are certainly unstable, it is sufficient to investigate only these two extreme cases. We begin with the "horizontal" disclination. To describe the field n, we make use of the formula (17) and expand the energy, i.e., the sum of the expressions (9) and (19), to squares of the small quantities θ and $\varphi_1 = \varphi - \varphi_0$, where φ_0 is the exact solution of the plane problem for $\alpha, \beta \neq 0$ (cf.[2]). As a result, for the second order terms we obtain an expression of the type $f_2 + \Delta f_2$, where f_2 is given by formula (10), and all terms linear in the small quantities α and β are collected in Δf_2. These arise both from the expansion of the expression (19) close to $\theta_0 = 0$, $\varphi_0 = n\chi/2$, and from the expansion of the second variation of (9) in a series in α and β. As before, the structure is again stable with respect to the variations φ_1 even in zeroth order in α and β. It is also clear that the eigenfunction for the "dangerous" eigenvalue has the form

$$\theta=\theta^*\sin(n\chi/2)+O(\alpha,\beta),$$

where $O(\alpha, \beta)$ are terms linear in α and β. It is clear that, to calculate the energy (the eigenvalue λ) to the same linear order in α and β, it is sufficient to calculate the integrals in Δf_2 with the functions $\varphi_1 = 0$ and $\theta_0 = \theta^* \sin(n\chi/2)$. The answer, naturally, is proportional to $\lambda\theta^{*2}$. By noting now that according to (18), on rotation of the plane through an angle θ^* we also have $\theta_0 = \theta^* \sin(n\chi/2)$ and $\varphi_1 \sim \theta^{*2} \to 0$, we conclude that $\lambda\theta^{*2}$ should coincide to within a numerical factor with the corresponding term of the expansion of (20) in a series in θ^*, inasmuch as both represent the correction to the energy of the "horizontal" disclination that is linear in α and β and due to the rotation of the plane of the disclination through an angle θ^*.

This completes the proof. It can also be carried through without difficulty for a "vertical" disclination, by repeating the above, word for word, for the energy defined now by the formulas (9) and (22) and for the director n described by formula (21), and replacing α and β by γ and δ, and θ^* by $\pi/2 - \theta^*$.

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