Surface disclinations in nematic liquid crystals
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SURFACE DISCLINATIONS IN NEMATIC LIQUID CRYSTALS

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Résumé. — On montre que, dans un cristal liquide nématique, les disclinations attachées aux limites de l'échantillon peuvent être traitées par un modèle du type Peierls-Nabarro connu de la théorie des dislocations dans les cristaux. Mathématiquement, les dislocations avec cœur plan et les disclinations sur la surface sont complètement analogues si on considère les approximations de l'élasticité isotrope et de la distribution planaire du directeur. Les solutions sont données d'abord pour les disclinations dans un demi-cylindre de grand rayon ; puis on discute la possibilité d'une asymétrie de la distribution du directeur sur la surface, qui peut être due à une asymétrie des forces d'ancrage. Les disclinations attachées à l'une des surfaces d'une couche nématique mince sont étudiées aussi. On montre que les conditions aux limites imposées par l'autre surface introduisent une asymétrie dans la distribution du directeur à l'intérieur de l'échantillon. Il faut distinguer cette asymétrie à longue distance de l'asymétrie intrinsèque à courte distance.

Abstract. — It is shown that in nematic liquid crystals the disclinations which are attached to the external boundaries of the specimens can be described by a Peierls-Nabarro type model known from the theory of crystal dislocations. Mathematically, dislocations with planar cores and surface disclinations are then completely analogous if the isotropic one-constant approximation and a planar distribution of the director are assumed. Solutions are first given for disclinations in a half-cylinder of large radius and the possibility of an asymmetry in the distribution of the director on the surfaces, which may be caused by an asymmetry in the anchoring forces, is discussed. Disclinations confined to one of the surfaces of a thin nematic layer are also studied. It is shown that the boundary conditions on the other surface may introduce an asymmetry into the distribution of the director in the bulk of the specimen. This long-range asymmetry should be distinguished from the intrinsic, short range asymmetry.

1. Introduction. — Disclinations are common defects encountered in liquid crystals. Their description generally requires both a topological study of the distribution of the director (for a review see [1]) and considerations of energy which have usually been based on the linear elastic theory of Oseen [2] and Frank [3]. In the case of a nematic liquid crystal the density of the elastic energy is

\[ f = \frac{1}{2} \left[ K_1 (\text{div } n)^2 + K_2 (n \cdot \text{curl } n)^2 + K_3 (n \times \text{curl } n)^2 \right] \] (1)

where \( n \) is the director (unit vector in the local direction of the molecules). The three terms represent splay, bend and twist respectively ; \( K_1, K_2, K_3 \) are the corresponding elastic constants. A great variety of disclinations are observed in different experiments. We shall distinguish here between defects which occur in the bulk of the specimen and those which are confined to external surfaces.

On the one-constant approximation

\[ (K_1 = K_2 = K_3 = K) \]

Frank [3] suggested the following planar solutions of the Euler equations of \( \int f \, dV \) for the twist and wedge disclinations in the bulk of the specimen :

\[ \theta = S \varphi + \theta_0 \] (2)

\( \theta \) is the angle between the director and a given axis, \( \varphi \) is the polar angle in a plane perpendicular to the disclination line and \( S \) is the strength of the disclination and is equal to either an integer or half-integer. (On a path around the line the inclination of the molecules changes by \( 2 \pi S \)).

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For the anisotropic case \((K_1 \neq K_2 \neq K_3)\) it was shown by Dzyaloshinkij [4] that the same planar solutions may be obtained for the wedge disclinations (with the exception of \(S = 1\)) but not for the twist disclinations. The solutions given by (2) are singular on the disclination line and give rise to the energy which diverges logarithmically on the line similarly as the elastic energy of crystal dislocations. However, for the case of integral strength \((S = \pm 1, \pm 2, \ldots)\) there is a possibility of completely removing the singularity by allowing the director to rotate slowly in the third dimension towards the direction of the disclination line. Such solutions have been worked out in detail by Cladis and Kléman [5] for the case of wedge disclinations and Meyer [6] has shown that this is also possible for twist disclinations. A similar possibility does not exist for half-integer disclinations whose director is always multivalued on the line. To study the core structure of these lines a microscopic molecular theory is needed. This basic difference between integral and half-integral disclination lines is to be related to the analogy between half-integer disclinated crystals and Moebius crystals. Hence two fundamentally different types of disclinations may exist in the bulk : coreless integer lines and half-integer lines which possess cores similar to dislocations in crystals. This classification applies not only to straight disclination lines but to any kind of disclination loop which may be of mixed wedge-twist character.

Surface defects were first observed and studied in detail by Friedel and Grandjean [7]. Their observations have been extended recently and systematized using the concept of a disclination [8, 9, 10] which was unknown to the former authors. These defects always lie in the interface between the liquid crystal with its supporting substrate (e. g. glass) and not on the free surface. The characteristic feature of these lines is that they are much wider than disclination lines in the bulk. This suggests that their core is spread on the surface. Another experimental feature is the asymmetrical distribution of the director sometimes observed in the vicinity of the line (9).

We define the strength \(\Sigma\) of a surface disclination as \(1/2\pi\) the difference \(\Delta\theta\) between the inclination of the director on either side of the disclination line measured on the surface far from the disclination. This definition allows for the existence of surface disclinations of any strength \(\Sigma = \Delta\theta/2\pi\); a complementary disclination of strength \(\Sigma_\pi\), defined by \(\Sigma + \Sigma_\pi = S\), where \(S\) is an integer or half-integer, is regarded as being virtual and outside the specimen. The disclination line of strength \(\Sigma \neq S\) is for example obtained when two misoriented microcrystallites melt into the nematic phase; such a line then appears on the surface at the common junction of the two crystallites, assuming that the anchoring boundary conditions are the same in both nematic and solid state (see Fig. 1). Since \(\Sigma\) may have any value \(\Delta\theta\) can be made very small and we are thus able to define a density of disclinations on a surface whilst such a concept has no clear meaning in the bulk. Consequently, disclination cores can always spread on a surface. In terms of the classification of disclination lines in the bulk this means that \(\Sigma_\pi\) can be chosen in such a way that \(\Sigma + \Sigma_\pi = n\), where \(n\) is an integer. In particular half-integer lines in the bulk can, in certain circumstances, attach themselves to the surface and their core singularity then disappears. There is, therefore, an energy barrier of topological origin resisting detachment of a disclination from the surface. It should be noted that this barrier is infinite when \(\Sigma\) is neither an integer nor half-integer, and that such a line cannot go into the bulk except by nucleation of other singularities (e. g. singular points).

The spreading of the disclination core on the surface is reminiscent of the Peierls [11] and Nabarro [12] model of a dislocation with planar core. In this model the crystal is treated as an elastic continuum but instead of the singular solution, a solution which corresponds to the dislocation being smeared into a continuous distribution of infinitesimal dislocations in its slip plane is found; the elastic energy does not therefore diverge on the dislocation line. Large inelastic displacements are confined to the slip plane and the character of the core smearing is determined from a balance between the elastic and restoring forces (which arise due to the interatomic interactions) on the plane of the spread (for a review see [13]).

Similarly, the core structure of surface disclinations may be regarded as determined by a balance between surface terms (arising from the anchoring energy) and bulk terms. The distribution of the director in the core is then determined by the dependence of the surface energy on the inclination, \(\theta\), of the director from the energetically most favourable direction.
In the present paper a model of the core structure of surface disclinations will be formulated in complete analogy with the Peierls-Nabarro model of dislocation cores. A simple analytical solution for the dislocation core structure in the original Peierls treatment [11] describes also the disclination core structure if a sinusoidal dependence of the surface energy on \( \theta \) is assumed; this solution is identical with that recently suggested by Meyer [14]. Solutions for a more general dependence of the surface energy on \( \theta \) will be discussed and the possibility of an intrinsically asymmetric core structure will be investigated. Finally the properties of surface disclinations with various core structures which lie on one of the surfaces of a thin nematic layer, which is the usual experimental situation, will be discussed in detail.

2. Peierls type model for surface disclinations. — In the following we shall use the isotropic one-constant approximation i.e. \( K_1 = K_2 = K_3 = K \). Planar rotation of the director defined by an angle \( \theta \) may then be assumed since planar solutions obey in this case de Gennes’ molecular field conditions [15] (see also [5]) and thus minimize totally the elastic energy.

The energy density given by eq. (1) reduces to
\[
f = \frac{1}{2} K (\nabla \theta)^2
\]
and the Euler equation for minimization of the total bulk energy is the Laplace equation
\[
\nabla^2 \theta = 0.
\]

Planar solutions and eq. (3) and (4) also hold for twist disclinations if \( K_1 = K_3 \neq K_2 \). The constant \( K \) in eq. (3) is then replaced by \( (K_1 K_3)^{1/2} \) and the coordinates in the plane of rotation have to be scaled accordingly [16]. These solutions, however, minimize the elastic energy under the condition of planarity only but not totally i.e. they do not satisfy de Gennes’ molecular field conditions.

Let us assume that the surface to which the disclination line is confined is the Oxy plane and that the disclination lies along the y axis; the rotation of the director may take place either in this plane or in a plane perpendicular to it. The balance of the forces on the surface leads to the condition
\[
\frac{dW_s(\theta)}{d\theta} = K \left( \frac{\partial \theta}{\partial z} \right)_{z=0} \quad (5)
\]
where \( W_s(\theta) \) is the surface energy of anchoring which is a function of \( \theta \). If the case \( K_1 = K_3 \neq K_2 \) is considered \( K \) is replaced by \( K_2 \) in eq. (5).

Eq. (5) is analogous to the condition for the balance of the elastic and restoring forces in the case of the Peierls model of a scalar dislocation [11]
\[
\frac{dy}{du} = \mu \left( \frac{\partial u}{\partial z} \right)_{z=0}
\]
where \( \gamma(u) \) is the energy of the fault created by displacing two halves of the crystal along the slip plane by an amount \( u \), where \( \mu \) is the shear modulus; \( dy/du = F(u) \) is usually called the restoring force [13]. In the bulk \( u \) obeys the Laplace equation \( \nabla^2 u = 0 \), and if the dislocation lies along the \( y \) axis
\[
u(x = +\infty, z) = 0 \quad \text{and} \quad u(x = -\infty, z) = b
\]
where \( b \) is the Burgers vector of the dislocation.

A complete analogy between the surface disclination and the Peierls dislocation is obtained if we identify different quantities as follows
\[
u \leftrightarrow \theta, \quad b \leftrightarrow 2 \pi \Sigma, \quad \gamma(u) \leftrightarrow W_s(\theta), \quad \mu \leftrightarrow K
\]
assuming that
\[
\theta(x = +\infty, z) = 0 \quad \text{and} \quad \theta(x = -\infty, z) = 2 \pi \Sigma
\]
which is equivalent to the above mentioned boundary condition for \( u \). This leads by comparison with the Peierls analysis [11] to the integral equation for \( \theta \) on the surface
\[
-\frac{dW_s}{d\theta} = K \int_{-\infty}^{+\infty} \frac{d\theta}{(x-x')^2} \frac{1}{z=0} x - x' \quad (8)
\]

We can interpret now \( (\partial \theta/\partial x')_{x'=0} \) as a disclination density, \( \rho(x') \), giving rise to the torque \( \frac{1}{\pi} \frac{1}{x-x'} \) at a distance \( |x-x'| \); in analogy with dislocations we shall call \( dW_s/d\theta = F(\theta) \) the surface restoring torque. The physical meaning of eq. (8) is then that the total elastic torque at a point \( x \) is balanced by the surface restoring torque i.e. by the torque due to surface anchoring. The general solution of eq. (6) which satisfies the boundary condition (5) or, equivalently, (8) is then
\[
\theta(x, z) = \frac{1}{\pi} \int \frac{z}{z^2 + (x-x')^2} \theta(x', z = 0) \, dx'.
\]
The total surface energy per unit length of disclination \( E_s = \int W_s(\theta) \, dx \) is independent of the functional dependence of \( W_s \) on \( \theta \) and is
\[
E_s = 2 \pi K \Sigma^2.
\]

This result is obtained by integration of \( \int W_s(\theta) \, dx \) by parts and using eq. (8); the same is true for the total core energy of a Peierls dislocation (see e.g. [17]).

In general the dependence of \( W_s \) on \( \theta \) is not known but for the case that \( \theta \) varies from 0 to \( \pi \) the simplest assumption is that
\[
W_s = W \sin^2 \theta \quad \text{and} \quad F_s = W \sin 2 \theta
\]
where \( W \) is a constant giving the maximum anchoring energy. For the case of \( \Sigma = \frac{1}{2} \) the eq. (8) and (9) yield a simple analytical solution
\[
\theta = \tan^{-1} \frac{z+s}{x}
\]
where \( s = K/2 W \) in conformity with the result of Meyer \[14\]. The Peierls' solution for the dislocation, 
\[ u = \frac{b}{\pi} \tan^{-1} \frac{z + \zeta}{x}, \]
obtained for the case that 
\[ dy/da = B \sin 2 \frac{\pi n u}{b}, \]
where \( B \) is a constant and 
\[ \zeta = \frac{b}{2 \pi B} \]
is obviously related to the solution (12) using relations (7). For \( \Sigma = n/2 \) where \( n \) is an integer larger than 1 the solution will be of the type

\[ \theta = \sum_{i=1}^{n} \tan^{-1} \frac{z + s}{x - x_i} \]

where \( x_i \to \pm \infty \) for \( i \neq 1 \). This means that a disclination of higher strength than \( 1/2 \) splits into disclinations of strength \( 1/2 \) and these repel each other. The solution (12) represents an asymmetrical core of the surface disclination.

The function \( \sin \theta(x, z) \) is only an approximation. In general the dependence of \( F_s(\theta) \) on \( \theta \) will be more complicated depending on both the kind of liquid crystal and the material used as substrate. In particular the substrate may introduce an asymmetry into the surface energy dependence on \( \theta \) so that \( F_s(\theta) \neq F_s(\pi - \theta) \) if we assume that \( 0 < \theta < \pi \). This would give rise to an asymmetry in \( \rho(x) \) and to an asymmetrical core of the surface disclination.

For a general surface restoring force a straightforward analytical solution usually cannot be found. However, methods of solving eq. (8) for any functional dependence of \( F_s(\theta) \) on \( \theta \) have recently been developed, in connection with the study of dislocation core structures, for restoring forces which are far from the sinusoidal dependence on displacement [18, 19, 20]. These methods are essentially iterative procedures for solving eq. (8) and could be directly applied to surface disclinations if a dependence \( F_s(\theta) \) is prescribed. The result of such calculations would give the distribution of the director on the surface i.e. \( \theta(x, z = 0) \); the distribution of the director in the bulk of the specimen has to be calculated using eq. (9). Since no measured dependences \( F_s(\theta) \) exist at present we shall not follow this line further and not solve eq. (8) for some hypothetical surface restoring torques. However we shall suggest a solution of eq. (4) which may represent a surface disclination with an asymmetrical core which corresponds to the type of the surface restoring force shown in figure 2a.

This solution of eq. (4) is

\[ \theta = A \phi \sin (b \phi + \alpha) + \theta^* \]  

where \( A, b, \alpha \) and \( \theta^* \) are constants and \( r \) and \( \phi \) cylindrical coordinates defined by the relations \( x = r \cos \phi, \) \( z = r \sin \phi \). Apparently eq. (15) cannot describe a disclination in the bulk since it creates a planar fault in the plane \( z = 0 \); it may, however, describe a disclination confined to the surface \( O_{xy} \). Assuming that the disclination lies along the \( y \) axis the constants \( A \) and \( \theta^* \) are determined from the conditions \( \theta = 0 \) for \( \phi = 0 \) and \( r = R \) and \( \theta = 2 \pi \Sigma \) for \( \phi = \pi \) and \( r = R \), where \( 2 R \) is the dimension of the specimen in the direction perpendicular to the disclination line. We then have

\[ A = \frac{2 \pi \Sigma}{R^2 \left[ \sin(b \pi \alpha + \alpha) - \sin \alpha \right]} \]

\[ \theta^* = \frac{2 \pi \Sigma \sin \alpha}{\sin(b \pi + \alpha) - \sin \alpha}. \]

In the following we shall only consider the case of \( \Sigma = \frac{1}{2} \). Eq. (15) generally corresponds to an asymmetrical distribution of the director in the plane \( O_{xy} \) i.e. \( \theta(x) \neq \pi - \theta(-x) \). However, a symmetrical distribution follows if \( \alpha = -bn/2 \). As will be shown below the values of \( b \) which are of interest lie in the interval \( 0 < b < 1 \). For those values of \( b \) eq. (15) represents a disclination with a singularity on the line since \( \theta(x, r) \to \infty \). The elastic energy per unit length of disclination, assuming the specimen
Asymmetrical restoring torque, $F_s$, given by eq. (19).

b) Corresponding density, $\rho$, of the continuous distribution of disclinations given by eq. (18) ($C_s = 4 \times 10^{-4}$, $p = 1.25$).

to be a half cylinder of radius $R$, is

$$E_{el} = \frac{1}{2} K A^2 b^2 \int_0^\pi d\varphi \int_0^R r^{2n-1} dr$$

which is not singular for this range of $b$, and is equal to

$$K \frac{\pi^3 b}{4[\sin(\beta \pi + \alpha) - \sin \alpha]^2}.$$ The elastic energy of disclinations described by eq. (15) will thus be relatively low when compared with disclinations described by eq. (2) since it does not diverge with the dimensions of the specimen, i.e. with $R$, or on the disclination line.

In order to remove the singularity on the disclination line we shall formally place the centre of the disclination outside the specimen i.e. we shall replace (15) by

$$\theta = A(x^2 + (z + s)^2)^{1/2} \sin(b \varphi + \alpha) + \theta_0$$

where $\varphi = \tan^{-1} \frac{z + s}{x}$ and $0 < s \ll R$. Physically this represents a continuous distribution of disclinations on the surface with the density

$$\rho(x) = (\partial \theta / \partial x)|_{z=0} = Ab(x^2 + s^2)^{1/2} \sin[(b - 1) \varphi_0 + \alpha]$$

with $\varphi_0 = \tan^{-1} s/x$. The surface restoring torque is then according to (5)

$$F_s(\theta(x)) =$$

$$K Ab(x^2 + s^2)^{(b-1)/2} \cos[(b - 1) \varphi_0 + \alpha].$$

(19)

It can easily be seen that both $\rho$ and $F_s$ are symmetrical only if $\alpha = -\frac{b \pi}{2}$ i.e. if $\theta(x)$ is symmetrical.

In the following we shall show that parameters $b$, $\alpha$ and $s$ can be chosen in such a way that (19) gives the surface restoring torques of the type shown in figure 2a.

Let us define

$$\tilde{F}_s = (F^\text{max}_s + |F^\text{min}_s|)/2$$

and $\rho = F^\text{max}_s/|F^\text{min}_s|$ where $F^\text{max}_s$ and $F^\text{min}_s$ are the maximum and minimum values of the surface restoring torque, respectively.

If we write

$$\tilde{F}_s = C_s \frac{K}{d}$$

(20)

where $d$ is a molecular length, $C_s$ may be expected to range from $10^{-4}$ to $10^{-2}$ [10]. We shall further assume that

$$F_s(\theta) = 0$$

$$\text{for} \quad \theta = \frac{2 \pi}{1 + p^2}$$

the surface restoring torque is zero for $\theta = \pi/2$ in the symmetrical case of $p = 1$. This condition is somewhat arbitrary and its variation will result in some variation of the surface restoring torque. For a given $p$ and $F_s$, we obtain the following three equations for $b$, $\alpha$ and $s$ :

$$F_s(\theta(x_{\text{max}})) = \frac{2 p}{1 + p} \tilde{F}_s$$

$$F_s(\theta(x_{\text{min}})) = \frac{2}{1 + p} \tilde{F}_s$$

$$F_s(\theta = \frac{2 \pi}{1 + p^2}) = 0$$

(21a, b, c)

$x_{\text{max}} = s/\tan(\varphi^\text{max}_0)$ and $x_{\text{min}} = s/\tan(\varphi^\text{min}_0)$ where $\varphi^\text{max}_0 = (\pi/2 + \alpha)/(2 - b)$ and $\varphi^\text{min}_0 = (3 \pi/2 + \alpha)/(2 - b)$ as follows from eq. 19 and from the condition for maximum and minimum of $F_s$, respectively. The eq. (21a-c) are transcendental and can only be solved numerically.

Numerical solutions of eq. (21a, b, c) have been found (using an iterative procedure) for $p = 1, 1.1, 1.25, 1.5$ and for various values of $C_s$. It was found that $b$ and $\alpha$ are practically independent of $C_s$, the value of which principally determines $s$. Furthermore $b$ is almost independent of $p$ so that one value of $b$, viz 0.163, could be used in all cases. The values of $\alpha$ corresponding to the above values of $p$ are respectively : $-0.0813 \pi$, $-0.0681 \pi$, $-0.0506 \pi$ and
The values of \(s\) range from \(1.2 \times 10^3\) for \(C_s = 10^{-4}\) to 5 for \(C_s = 10^{-2}\). The dependence of the calculated quantities on the size of the specimen, characterised by \(R\), is very weak and can be neglected if \(R\) is sufficiently large (in the present calculations \(R = 5 \times 10^6\) was used; assuming that \(d \approx 20\) Å, \(R = 1\) cm).

Reasonable surface restoring torques can be obtained for \(C_s < 10^{-3}\) and figure 2a shows \(F_s(\theta)\) for \(C = 4 \times 10^{-4}\) and \(p = 1.25\); the corresponding density of disclinations given by eq. (18) is shown in figure 2b. For \(C_s > 10^{-3}\) the values of \(\theta\) for which the maximum and minimum values of \(F_s(\theta)\) occur, come very close to each other and they differ by only \(\sim 2^\circ\) for \(C_s = 10^{-2}\); this type of the dependence of the surface restoring torque on \(\theta\) does not seem physically reasonable. The elastic energy per unit length of this surface disclination in the half cylinder of radius \(R\) is

\[
E_{el} = \frac{1}{4} KA^2 b^2 R^{2b} \times
\left[ (\pi - 2 \varphi_1) - \left( \frac{s}{R} \right)^{2b} \int_{\varphi_1}^{\pi} \frac{1}{\sin^{2b} \psi} d\psi \right]
\]

where \(\varphi_1 = \tan^{-1} \frac{s}{R}\). The surface energy is, of course given by (10). For \(R = 5 \times 10^6\) the total energy \(E = E_{el} + E_s\) was calculated as a function of \(C_s\) and the result is shown in figure 3; since the energy was found to be almost independent of \(p\) only the case of \(p = 1.25\) is plotted. For the symmetrical restoring force given by (11) we can put \(W = C_s K A^2 d\).

The total energy of the disclination described by (12) can be calculated as a function of \(C_s\) using eq. (14); this dependence is also plotted in figure 3 for the same value of \(R\). It is seen that the energy of the disclination described by (12) is for a given value of \(C_s\) always higher than the energy of the disclination described by (17). We cannot conclude, however, that the type (17) disclination is energetically more favourable than the type (12) since it is the dependence of the surface restoring force on \(\theta\) which decides the spread of the disclination core and thus also the solution in the bulk.

4. Surface disclinations in thin nematic layers. — The samples of liquid crystals are usually prepared in the form of thin layers for example as small flat droplets on a glass surface or on a crystal cleavage plane, layers in between two glasses etc. We shall, therefore, study the surface disclinations lying on one of the surfaces of a nematic layer of thickness \(h\). The disclinations will be assumed to be on the bottom surface \(Oxy\) lying along the \(x\) axis; both disclinations of the types described by eq. (12) and (17) will be considered. On the other surface \(z = h\) a fixed inclination, \(\beta\), of the director will be assumed i.e. the boundary condition

\[
\theta(x, z = h) = \beta
\]

where \(0 < \beta < \pi/2\), will be imposed. This may correspond for example to the nematic layer in between two rubbed glasses (the direction of rubbing determines the preferential direction of the molecules) when the top glass was rotated with respect to the bottom one by the angle \(\beta\), or to a droplet when the molecules on the free surface are strongly anchored and inclined at the angle \(\beta\) to the surface. The disclination free specimen is then deformed by a constant bend or twist i.e. \(\theta = \beta \frac{z}{h}\) in the undisclination sample.

The solutions which give the same distributions of the director on the surface \(Oxy\) as those given by (12) or (17) and satisfy both eq. (4) and boundary condition (22) can be readily obtained using the method of images. The case of the type (12) we obtain

\[
\theta = \lim_{N \to \infty} \sum_{n = -N + 1}^{N} \theta_n + \frac{\pi}{2} \left( 1 - \frac{z}{h} \right) + \beta \frac{z}{h}
\]

where

\[
\theta_n = \tan^{-1} \frac{z - 2 nh + s}{x}
\]

where the plus sign applies for \(n \leq 0\) and minus sign for \(n > 0\). In the case of the type (17) disclination the corresponding solution is

\[
\theta = \lim_{N \to \infty} \left[ \sum_{n = -N + 1}^{N} \theta_n - \theta_n^\# + \theta_n^\# \frac{z}{h} \right] +
\]

\[
+ \theta^\# \left( 1 - \frac{z}{h} \right) + \beta \frac{z}{h}
\]

where

\[
\theta_n = A(x^2 + (z - 2 nh + \delta)^2)^{1/2} \times
\]

\[
\times \sin \left( b \tan^{-1} \frac{z - 2 nh + s}{x} + \alpha \right) \text{ for } n \leq 0
\]
and \( \theta^* \) is given by (16).

However, if the surface restoring torques depend on \( \theta \) according to (11) and (19), respectively, the solutions (23) and (24) do not satisfy eq. (5) which represents a boundary condition on the bottom surface. It can be shown, however, that if the thickness of the specimen is large enough the deviation from this condition is small. For the case described by eq. (23) we obtain

\[
K \left( \frac{\partial \theta}{\partial z} \right)_{z=0} = K \lim_{N \to \infty} \sum_{n=1}^{N} \frac{x}{x^2 + (2nh \mp s)^2} + K \left( \frac{\beta - \pi}{2} \right) \frac{1}{h},
\]

Assuming (11) the condition (5) is obviously satisfied by the term in the summation which corresponds to \( n = 0 \). The other terms in the sum and the constant term will not be important if their absolute value is much smaller than \( W \). Since \( s \ll h \) we can write the rest of the sum as

\[
2 K \sum_{n=1}^{\infty} \frac{x}{x^2 + 4n^2h^2} \text{ and because } \left| \sum_{n=1}^{\infty} \frac{q}{q^2 + n^2} \right| \leq \frac{\pi}{2}
\]

for any finite \( q \) the absolute value of the rest of the sum is \( \leq K \frac{\pi}{2} \). At the same time the maximum value of the constant term is \( K \frac{\pi}{2} \) and thus the condition mentioned above will be satisfied if \( K \frac{\pi}{2h} \gg W \).

Using (11) and (20) we obtain then \( h \gg \frac{d}{C_\alpha^2} \).

Obviously the thickness of the sample for which this condition is satisfied depends on \( C_\alpha \); assuming \( d \approx 20 \text{ Å} \) then for \( C_\alpha = 10^{-4}, h \gg 10^3 \text{ Å} \) while for \( C_\alpha = 10^{-2}, h \gg 10^5 \text{ Å} \). The usual thickness of the specimens used in experimental studies is more than \( 10^6 \text{ Å} \) [9, 10] and therefore the required conditions will be satisfied. Similar reasoning can be carried out for the case of eq. (24) but the series has to be discussed term by term. For the value of \( h \) found in §3 the condition for \( h \) is very much the same as in the case of eq. (23). For the thickness of the samples usually encountered in experiments solutions (23) and (24) can thus be regarded as good approximations to the solutions which would satisfy the boundary conditions on both the top and bottom surfaces exactly.

The elastic energy per unit length of the disclination

\[
E_{el} = \frac{1}{2} K \int (\nabla \theta)^2 \, dx \, dz
\]

can be written in the form of a number of double integrals when using (23) and/or (24). The corresponding formulae are rather complex and will not be listed here. The surface energy is again given by eq. (10). The total energy per unit length of a disclination

![Fig. 4. Total energy, \( E \), of a surface disclination in a nematic layer as a function of \( C_\alpha \) for different angles \( \beta \). a) Disclination of type (23). b) Disclination of type (24). c) Variation of energy density in the vicinity of a line introduced in a distorted medium.](image)
nation in the nematic layer of thickness $h$ was calculated as a function of $C_\perp$ (see eq. (20)) for four different values of $\beta : 0^\circ$, $45^\circ$, $75^\circ$ and $90^\circ$. The calculations were made for disclinations described by (23) and by (24); in the latter case the same parameters $b$, $a$ and $s$ as in the previous paragraph, were used. Since the disclination free specimen is deformed by a constant bend or twist due to the boundary condition on the top surface, its energy is assumed to be $K_\delta^2 \frac{R}{h}$. The computations were carried out numerically using Romberg's integration method [21]. The dimension of the specimen perpendicular to the disclination line was chosen to be $2R = 200h$ (for $h = 100 \mu$, $R = 1$ cm) but for such large $R$ the results are practically independent on this quantity. A finite number of images, $N$, was used in numerical calculations; $N$ was always chosen in such a way that on the bottom surface the deviations of the director from the prescribed values were not more than $\pm 5^\circ$. The results of these calculations are shown in figure 4a for the case (23) and in figure 4b for the case (24) for $\rho = 1.25$. An interesting feature now occurs in contrast to similar dependences shown in figure 3. For large angles of $\beta$ the total energy may be small or even negative. This is illustrated figure 4c where we have plotted as an example the quantity $\sigma - \sigma_0$ versus $x/h$ for $z = 0.5h$. Here $\sigma$ is the density of energy in the disclinated medium and $\sigma_0$ the density before introducing the disclination, for $\beta = 75^\circ$ and $\rho = 1.25$. We notice a strong decrease in the vicinity of the disclination, which is large enough to overcome the increase in twist (or bend) in the region $x < 0$. If we look at other values of $z/h$, we would notice that this decrease in energy would be larger for small values of $z/h$ (near the disclination line) and can therefore compensate the surface energy, whereas for large values of $z/h (\approx 1)$ the decrease is small but the density $\sigma - \sigma_0$ is smaller than for $z/h \approx 0$. In conclusion, the introduction of a surface disclination changes very little or may even decrease the elastic energy of the specimen which was deformed originally by a constant bend or twist. Remember that this calculation is done for a finite specimen. The less realistic case of an infinite specimen with an isolated line would of course always lead to a positive energy.

The distribution of the director near the core of a surface disclination is shown in figure 5a for a disclination of the type (23) and in figure 5b for the type (24); in the latter case $\rho = 1.25$. These figures correspond to $\beta = 45^\circ$ but practically the same picture is obtained for any value of $\beta$. The distribution of the director in the bulk of the specimen is practically the same for the type (23) and for the type (24) disclination and it is shown in figures 6 and 7 for $\beta = 45^\circ$ and $90^\circ$, respectively. For all figures $C_\perp = 4 \times 10^{-4}$ was assumed but the distributions are similar for other values of $C_\perp$. The director at different points in the $Oxz$ plane is depicted as a short oriented line the length of which is proportional to $\cos \theta$ and scaled so as to run from one mesh point to the other if $\theta = 0$ or $\pi$. It should be noted that the rotation takes place in the plane of the picture for wedge disclinations and is perpen-
cular to the picture for twist disclinations. It is seen that in the disclination core the distribution of the director is different for the two types of disclinations and it is practically independent of the boundary condition on the top surface; in particular in figure 5b an asymmetrical distribution on the bottom surface is seen. On the other hand, the distribution of the director in the bulk is very similar for both types of disclinations and its features are principally determined by the boundary conditions on the top surface. The bulk distribution of the director is asymmetrical even in the case of the symmetrical core and an extrinsic asymmetry is thus introduced.

5. Conclusions. — Surface disclination lines in nematics have been treated in this paper using a concept known in the theory of crystal dislocations as the Peierls-Nabarro model of the dislocation core. A complete analogy between dislocations with planar cores and surface disclinations has been established in the isotropic case; we had only to replace displacements by rotations and stresses by torques. An extension to the anisotropic case would certainly be possible since the definition of the disclination density, which is a fundamental physical concept in this model, is geometrical in nature. The present calculations are, however, restricted to the isotropic case and furthermore only to planar rotations of the director, i.e. a depending on only one angular variable. The latter restriction is not too far from reality for all situations where the anchoring conditions are such that the director stays tangent to parallel glass plates; this induces mostly twist because $K_2$ is the smallest elastic constant in all known nematics.

The following features of surface disclinations as revealed by the model, can be expected not to depend sensitively on the above mentioned approximations:

(i) The distribution of the director in the vicinity of the disclination line is non-singular.

(ii) The core region in which the orientation of the director varies rapidly with position extends over a distance $\sim W/K$, where $W$ is the maximum restoring torque.

(iii) The boundary conditions on all surfaces limiting the specimen, not only the surface containing the disclination line, have to be taken into account when determining the distribution of the director in the bulk of the specimen. In particular, in the case of flat nematic layers, a fixed inclination of the director on the surface which does not contain the disclination, may cause an asymmetric distribution of the director in the bulk. This external asymmetry may occur as a cholesteric type layer on one side of the disclination line (see Fig. 6). An intrinsic asymmetry can be introduced by the boundary conditions on the surface which contains the disclination, by asymmetrical anchoring conditions. However, this asymmetry spreads only over a distance comparable with the width of the core. For the values of $W/K$ used in this paper, which are reasonable for the experiments described in [9, 10], this spread is too small for the resolving power of the polarizing optical microscope. The asymmetry in the distribution of the director observed near some surface disclinations in [9] has to be attributed, therefore, to the influence of external boundaries. Intrinsically asymmetric disclination cores may be expected for samples with various crystalline substrates (cleavage planes), but a higher resolution than that available in the optical microscope is needed for the observation of this asymmetry.

References


