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Twist Disclinations in Elastically Anisotropic Nematic Liquid Crystals

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The influence of elastic anisotropy on twist disclinations in nematic liquid crystals has been considered. It is shown that anisotropy alters the structure as well as the energy of disclinations. The problem is exactly solvable when there is twist anisotropy only, i. e., $K_{11} = K_{33} \neq K_{22}$. When there is pure splay-bend anisotropy one can get the leading corrections to the structure and energy through a perturbation technique. The properties of twist and wedge disclinations in the presence of anisotropy have also been compared. Elastic anisotropy influences $+s$ and $-s$ disclinations differently in the case of wedge disclinations, but not so in the case of twist disclinations. For pure splay-bend anisotropy, twist disclinations have, in general, a higher energy than wedge disclinations. This may partly account for the absence of twist disclinations in nematic liquid crystals.

INTRODUCTION

Two types of disclinations are possible in nematic liquid crystals.[1,2] In the wedge type of disclination the line of singularity is perpendicular to the plane in which the molecules lie. The schlieren texture exhibited by nematics is due to such defects. In the second type of disclination the line of singularity is in the plane in which the molecules lie. In the literature this has been referred to as the *twist disclination.* Such disclinations have not been seen in nematics, but they appear as Grandjean-Cano lines in cholesterics.

The structure and properties of wedge disclinations are quite well established both theoretically and experimentally.[1-4] More recently the effects of elastic anisotropy on such disclinations have also been considered.[4-6]

Elastic anisotropy alters the structure profoundly.[3-5] The director pattern of a defect of any given strength s is not at all easy to obtain, and it is only in the extreme case of very small or very large elastic anisotropy can one hope to get analytical solutions. In general, however, it can be obtained numerically. This is largely due to the strong nonlinear terms in the equation of elastic equilibrium. Yet interestingly for $s = +1$ and $s = +2$ isotropic solutions continue to hold irrespective of the strength of the anisotropy.

The problem of disclination interaction is also altered significantly due to anisotropy. Firstly one has the radial interaction between defects which accounts for the familiar disclination reactions. The computation of the force of radial interaction is a formidable problem unless one makes use of the scaling properties of the differential equation of equilibrium.[5] If $\phi(x, y)$ is the solution for any given separation d between defects, then $\phi(x/\lambda, y/\lambda)$ is also a solution and this corresponds to a separation λd between defects. Employing this procedure one can reduce the force of interaction to the computation of integrals involving single defect solutions. Again the force of interaction as in a single constant case varies inversely as the distance of separation.

In addition, there is one other remarkable consequence of anisotropy. A new type of interaction comes into play.[6] In the isotropic case, the energy is independent of the relative orientations of the disclinations, but this is no longer true in the presence of anisotropy and only certain orientations are energetically allowed. Any deviations from these orientations will bring in angular forces. To a first order in elastic anisotropy one can compute this angular force using isotropic solutions.[6] This new type of disclination interaction completely alters disclination couplings in twisted nematics and long pitched cholesterics. In the elastically isotropic medium, be it nematic or cholesteric, one can have a pair of straight parallel disclinations, the difference in the case of the cholesteric being that the pattern is subject to a continuous alteration as we go along the axis of twist. But a change of pattern costs energy if we bring in elastic anisotropy. In this case the pattern would prefer to be the same in every cholesteric layer. Thus, pairs of disclinations will have to be coiled to minimize energy. This is in fact supported by the experimental observations of Rault[7] and Cladis *et al.*[8]

On the other hand twist disclinations do not appear to have attracted much attention. In view of the interesting consequences of elastic anisotropy in the case of wedge disclinations, we consider a similar situation for twist disclinations. When there is only the anisotropy of twist, i.e., $K_{11} = K_{33} \neq K_{22}$ one can rigorously solve the problem. However, in the presence of pure splay-bend anisotropy, i.e., $K_{11} \neq K_{33}$, $K_{22} = (K_{11} + K_{33})/2$, one has to invoke a perturbation technique. To simplify the problem it is throughout assumed that all distortions in the anisotropic medium are planar.

THEORY

We look for solutions with disclination along the Z-axis and the director in the ZX plane:

$$n_x = \cos\phi, \quad n_y = 0, \quad n_z = \sin\phi, \quad \phi = \phi(x, y), \tag{1}$$

which in cylindrical polar (r, α) can be expressed by

$$n_r = \cos\phi\cos\alpha, \quad n_\alpha = -\cos\phi\sin\alpha, \quad n_z = \sin\phi \tag{2}$$

$$\alpha = \tan^{-1} y/x, \quad \phi = \phi(r, \alpha)$$

The elastic free energy density is given by

$$F = \tfrac{1}{2}[K_{11}(\nabla\cdot\mathbf{n})^2 + K_{22}(\mathbf{n}\cdot\nabla\times\mathbf{n})^2 + K_{33}(\mathbf{n}\times\nabla\times\mathbf{n})^2]. \tag{3}$$

K_{11}, K_{22} and K_{33} are respectively splay, twist and bend elastic constants.

If ϕ is a function of α only this reduces to

$$F = \frac{\phi_\alpha^2}{2r^2}[K_{11}\sin^2\phi\sin^2\alpha + K_{22}\cos^2\alpha + K_{33}\cos^2\phi\sin^2\alpha], \tag{4}$$

where

$$\phi_\alpha = d\phi/d\alpha.$$

(I) $K_{11} = K_{22} = K_{33} = K$, (Elastic Isotropy)

In the one constant approximation:

$$F = \frac{K}{2}\frac{\phi_\alpha^2}{r^2} \tag{5}$$

and the equation of equilibrium is

$$\phi_{\alpha\alpha} = 0. \tag{6}$$

This gives the following simple solutions for the twist disclinations:

$$\phi = s\alpha + C = s\tan^{-1}\frac{y}{x} + C \tag{7}$$

$s = \pm\frac{1}{2}N (N = \text{integer})$, C = constant. The net elastic energy given by

$$E = \iint F\, r dr d\alpha$$

reduces to

$$E = \pi K s^2 \ln \frac{R}{r_c}. \tag{8}$$

R is the sample dimension and r_c the core radius. It is seen that $+s$ and $-s$ solutions are not structurally different but for a mirror $Y \leftrightarrow -Y$, about the $Y = 0$ plane. In this respect it differs markedly from wedge disclinations where $+s$ and $-s$ have totally different structures. Nevertheless the energy is independent of the sign of s and is equal to that for a wedge disclination of the same $|s|$. However, in contrast to the case of wedge disclinations, in which the constant C plays a minor role (of the rotation of the coordinate system excepting in the case of $s = +1$), here different values of C yield different structures of the same strength s. The equation of equilibrium for a collection of singularities becomes

$$\phi_{xx} + \phi_{yy} = 0.$$

This admits solutions of the type

$$\phi = \sum_i s_i \tan^{-1} \frac{y - y_i}{x - x_i} + C.$$

In other words, the superposition principle is valid. In this respect also twist disclinations are indistinguishable from wedge disclinations. Thus in an elastically isotropic nematic, twist disclinations have the same probability of existence, energetically, as wedge disclinations.

It should be mentioned here that Kleman[9] has suggested another possible model for a twist disclination wherein the director suffers a twist all round the singular line—a radial twist disclination. It is easy to show that $n_r = \cos\phi$, $n_\alpha = 0$, $n_z = \sin\phi$, with $\phi = s\alpha + C$ is *not* an allowed solution of the equation of equilibrium. Bouligand[10] has suggested a different solution. Here as one traces a loop in the horizontal plane the director rotates both about the vertical as well as a horizontal axis. Both rotations are proportional to the polar angle about the vertical axis. This again is *not* allowed by the equation of equilibrium.

Finally, it should be noticed that between crossed polaroids twist disclinations do not yield brushes. They should appear as lines surrounded by a more or less uniform field of view.

(II) $K_{11} = K_{33} \neq K_{22}$ (Twist anisotropy only)

The free energy density for this case is:

$$F = \frac{K}{2}(\phi_x^2) + \frac{K_{22}}{2}\phi_y^2$$

$$= \frac{K}{2}[\phi_x^2 + \Delta^2\phi_y^2] \quad \Delta^2 = K_{22}/K \tag{9}$$

And the equation of equilibrium is:

$$\frac{\partial^2\phi}{\partial x^2} + \Delta^2\frac{\partial^2\phi}{\partial y^2} = 0 \tag{10}$$

This gives the following simple director field:

$$\phi = s\tan^{-1}\frac{y}{\Delta x} + C \quad s = \pm\frac{N}{2} \tag{11}$$

The energy of the disclination $E = \int F\,dx\,dy$ is given by

$$E = \pi K s^2 \Delta \ln\frac{R}{r_c}$$

$$= \pi s^2\sqrt{KK_{22}}\ln\frac{R}{r_c} \tag{12}$$

It follows from this that for $K_{22} < K$ the twist disclination is more stable than the wedge disclination, while for $K_{22} > K$ the reverse is true.

It is interesting that Eq. (10) allows solutions of the type

$$\phi = \sum_i s_i\tan^{-1}\frac{y - y_i}{\Delta(x - x_i)} + C \tag{13}$$

Thus the superposition principle again works rigorously excepting that the x coordinate is scaled by a factor of Δ.

One consequence of this is that the net energy as well as the interaction energy of a pair disclinations (for the same separation between them) becomes a function of α. In other words one finds an anisotropy in the interaction between any two disclinations and energetically a particular angle, $\alpha_O = 0$ or $\pi/2$, yields a configuration of minimum energy.

(III) Splay-Bend anisotropy

$$K_{11} \neq K_{33} \text{ and } K_{22} = \frac{K_{11} + K_{33}}{2} = K, \quad \epsilon = \frac{K_{11} - K_{33}}{K_{11} + K_{33}}$$

In this case the free energy density becomes

$$F = \frac{K}{2} \frac{\phi_\alpha^2}{r^2} (1 - \epsilon \sin^2 \alpha \cos 2\phi) \tag{15}$$

The equation of equilibrium

$$\frac{d}{d\alpha}\left(\frac{\partial F}{\partial \phi_\alpha}\right) - \frac{\partial F}{\partial \phi} = 0 \tag{16}$$

reduces to

$$\phi_{\alpha\alpha} = \epsilon\, [(\sin^2 \alpha \cos 2\phi)\phi_{\alpha\alpha} + (-\sin^2 \alpha \sin 2\phi)\phi_\alpha^2 + (\sin 2\alpha \cos 2\phi)\phi_\alpha] \tag{17}$$

When $\epsilon = 0$ we get the unperturbed solution

$$\phi_0 = s\alpha + C \quad s = \pm N/2, \quad N = \text{integer.}$$

When $\epsilon \neq 0$ and small we can employ a first order perturbation solution

$$\phi = \phi_0 + \epsilon\psi \tag{18}$$

Then

$$\psi_{\alpha\alpha} \approx -\phi_{0\alpha}^2 \sin^2 \alpha \sin 2\phi_0 + \phi_{0\alpha} \sin 2\alpha \cos 2\phi_0 \tag{19}$$

which can be integrated to yield for $s \neq \pm 1$

$$\psi = A + \psi_0$$

$$\psi_0 = (\tfrac{1}{8}) \sin 2(s\alpha + C) + \left[-\frac{s(s+2)}{16(s+1)^2}\right] \sin 2\,[(s+1)\alpha + C] + \left[-\frac{s(s-2)}{16(s-1)^2}\right] \sin 2\,[(s-1)\alpha + C] \tag{20}$$

For $s = \pm 1$ one finds

$$\psi_0 = \frac{1}{8} \sin 2(\alpha s + C) - \frac{3}{64} \sin 2(2\alpha s + C) \tag{21}$$

And up to second order in ϵ the free energy density (for any s) is

$$F = \frac{K}{2r^2}\{s^2 + \epsilon[2s\psi_{0\alpha} - s^2 \sin^2\alpha \cos 2(\phi_0 + A)] + \epsilon^2[2s^2\psi_0 \sin^2\alpha \sin 2(\phi_0 + A) - 2s\psi_{0\alpha} \sin^2\alpha \cos 2(\phi_0 + A) + \psi_{0\alpha}^2]\} \quad (22)$$

RESULTS

In the case of half singularities one can show from Eqs. (20) and (22) that there is no first order correction to the one-constant energy given by Eq. (8), while the second order correction is independent of the sign of s and is

$$\Delta E = \frac{1}{4}\left[\frac{\pi K}{2} \ln R/r_c \cdot\right]\cdot \epsilon^2 g,$$

where

$$g = -\frac{142}{288}\cos 2A + \frac{3}{8}\cos(4C + 2A) - \frac{3}{16}\cos 4C + \frac{142}{576}.$$

Interestingly ΔE depends on both A and C and has the lowest value when $A = 0, \pm\pi \ldots$ and $C = \pm\pi/4, \pm 3\pi/4 \ldots$ This minimum value of ΔE is given by

$$\Delta E_{min} = -\frac{\pi K \epsilon^2}{8}\left(\frac{250}{576}\right) \ln R/r_c$$

i.e.,

$$\Delta E_{\min} \cdot \left(\pm \frac{1}{2}\right) - \pi K \epsilon^2 \left(\frac{0.87}{16}\right) \ln R/r_c \quad (23)$$

On the other hand in the case of wedge disclinations one finds[4] for $s \neq +1$ or $+2$

$$\psi_0 = \frac{s(2 - s)}{4(s - 1)^2} \sin 2[(s - 1)\alpha + C] \quad (24)$$

and

$$\Delta E_{\min} = -\frac{\pi K \epsilon^2}{2}\left[\frac{s^2(2 - s)^2}{4(s - 1)^2}\right] \ln R/r_c \quad (25)$$

which gives

$$\Delta E_{\min}\left(+\frac{1}{2}\right) = -\pi K\epsilon^2\left(\frac{4.5}{16}\right)\ln R/r_c$$
$$\Delta E_{\min}\left(-\frac{1}{2}\right) = -\pi K\epsilon^2\left(\frac{1.4}{16}\right)\ln R/r_c \tag{26}$$

We conclude from Eqs. (23) and (26) that wedge disclinations have a smaller energy than twist disclinations.

In the case of $s = \pm 1$ twist disclinations from Eqs. (21) and (22) we find a first order contribution to the one-constant energy Eq. (8) and it is

$$\Delta E(\pm 1) = \left(\frac{\pi K}{2}\right)\epsilon \cos 2\,(A + C)\ln R/r_c, \tag{27}$$

whose minimum value is

$$\Delta E_{\min}(\pm 1) = -\frac{\pi}{2}\,\epsilon\, K \ln R/r_c.$$

On the other hand for wedge +1 disclinations,

$$\Delta E_{\min}(+1) = -2\pi\,\epsilon\, K \ln R/r_c$$

and for −1 the correction is of second order in ϵ. Thus for $s = +1$ also twist disclinations have higher energy than wedge disclinations. One can conclude that in general it is energetically unfavorable for twist disclinations to exist in nematics. This may be one of the reasons why we do not see them in nematic liquid crystals.

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