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On Dislocations in Cholesteric Liquid Crystals

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The coarse-grained approximation has been used to work out the structure and properties of dislocations in cholesteric liquid crystals. In this model, edge dislocations are like smectic A edge dislocations while screw dislocations are like nematic wedge disclinations. Thus, it turns out that as regards their energies, interactions, and slow motions, the two types of dislocations behave quite differently.

1. INTRODUCTION

Cholesteric liquid crystals are characterized by a helical stacking of nematic-like layers. However, one frequently finds defects in this type of ordering.[1] The nature and properties of these defects have been studied both experimentally and theoretically.[2-5] Two of the well established defects are screw and edge dislocations.

Screw dislocations have their singularity along the helix axis and as one goes round this line, one finds the director orientation to change by an integral multiple of π. In the case of edge dislocations one has the singular line perpendicular to the helix axis, i.e. it is parallel to the cholesteric planes. On going round this line one gains an integral number of half pitches.

The details of the director pattern in the neighborhood of these dislocations have also been worked out. In both cases, the director is confined to the cholesteric plane, i.e. normal to the helix axis. For screw dislocations, the pattern is[3]

$$\mathbf{n} = \begin{bmatrix} \cos\varphi \\ \sin\varphi \\ 0 \end{bmatrix}, \quad \varphi = s \tan^{-1}\frac{y}{x} + q_0 z \tag{1}$$

where $2\pi/q_0$ is the pitch of the cholesteric, and the defect free sample has its helix axis along the z-direction. In the case of edge dislocation, the director pattern is given to a good approximation by[2]

$$\mathbf{n} = \begin{bmatrix} \cos\varphi \\ \sin\varphi \\ 0 \end{bmatrix}, \quad \varphi = s \tan^{-1}\frac{z}{x} + q_0 z \tag{2}$$

In either case, s signifies the strength of the defect which can take positive or negative integral or half integral values, being $\pm\frac{1}{2}$ for the dislocations of least energy.

We see from Eq. (1) and Eq. (2) that cholesteric, screw, and edge dislocations are respectively exactly like the wedge and the twist disclinations in nematics excepting for a superimposed twist $q_0 z$. Thus, they will simulate them as regards their energetics and interactions.

However, in many experimental situations we find cholesterics to exhibit smectic A like behavior. Focal conic textures in cholesterics are quite common.[1] Both smectic A and cholesterics exhibit Helfrich instabilities[6] resulting in a square grid pattern under the influence of an external magnetic field or a mechanical strain.[7] At low shear rates both have enormous viscosities being a million times what one finds in the high shear region.[8] All these phenomena can be explained using the coarse grained approximation,[9-11] where the distortions are supposed to be slowly varying in space. In this model the cholesteric behaves as though it is made up of layers (of thickness $P_0/2$) which preserve their identity. Again, theoretically, it has been predicted[12] that on this model, the cholesterics must have further analogies with smectic A. The mean squared amplitude of layer fluctuations induced by temperature should diverge logarithmically as sample size. Also, one must find second sound propagation in directions not exactly coinciding with the helix axis or its normal. In view of these facts, it is tempting to propose that dislocations in cholesterics are like those in smectic A. In fact, topologically, Bouligand[4] has indicated this possibility. However, the important consequences of this, as regards the energies and interactions, does not appear to have been noticed. This paper discusses this problem of defects in the coarse grained approximation. We compare and contrast the solutions with those of nematics and smectic A. We find the interesting result that the screw dislocation in this model is exactly like the wedge disclination in nematics described by Eq. (1). The edge dislocations on the other hand are exactly like edge dislocations in smectic A which are entirely different from what Eq. (2) describes. In fact, in this new model of edge dislocation, one can have clustering of like dislocations to form low angle grain boundaries. It is because of these differences that

screw and edge dislocations behave very differently when they are in slow motion. The frictional force for screw dislocations is proportional to the square of its strength s, while it is proportional to the strength itself for edge dislocations.

2. THEORY

The free energy density of elastic deformations in a cholesteric is given by

$$F_0 = \frac{1}{2}[K_{11}(\nabla \cdot \mathbf{n})^2 + K_{22}(q_0 + \mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_{33}(\mathbf{n} \times \nabla \times \mathbf{n})^2] \quad (3)$$

Here K_{11}, K_{22}, and K_{33} are the splay, twist, and bend elastic constants respectively. The equation of equilibrium which gives us allowed static distortions is

$$\frac{\partial}{\partial x_j}\left(\frac{\partial F_0}{\partial n_{i,j}}\right) - \frac{\partial F_0}{\partial n_i} = 0 \quad (4)$$

where $n_{i,j} = \partial n_i / \partial x_j$.

If one were to look upon a cholesteric as a stack of layers each of thickness $P_0/2$, then the energy density of elastic deformations in terms of layer displacement u along the layer normal is given by

$$F = \frac{1}{2}B\left(\frac{\partial u}{\partial z}\right)^2 + \frac{1}{2}\bar{K}\left[\left(\frac{\partial^2 u}{\partial x^2}\right) + \left(\frac{\partial^2 u}{\partial x^2}\right)\right]^2 \quad (5)$$

the first term represents the layer dilatation and the second term curvature in the layers. The assumption implied in Eq. (5) is that distortions u are gradual and slow in comparison with the pitch P_0. Within the framework of this model, we find from Eq. (3) and Eq. (5)

$$\begin{aligned} B &= K_{22}q_0^2 \\ \bar{K} &= \frac{3}{8}K_{33} \end{aligned} \quad (6)$$

And the equation of equilibrium obtained by minimizing Eq. (5) is

$$\lambda^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)^2 u = \frac{\partial^2 u}{\partial z^2} \quad (7)$$

where $\lambda = \sqrt{\bar{K}/B}$. We thus can see the complete analogy with smectic A (with a layer thickness $= P_0/2$).

In this analysis of cholesteric deformations, the following singular solutions are allowed.

a. Edge dislocations

Let the layers be in the xy plane, and the line of singularity along y. Then the distortions u in the vicinity are given by[15,14]

$$u(x, z) = \frac{P_0}{8}\left\{1 + \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{dk}{ik}\exp[-\lambda k^2|z| + ikx]\right\} \tag{8}$$

From this one can easily get the layer tilt $\theta = \partial u/\partial x$ (with reference to z axis) and layer dilatation $\delta = \partial u/\partial z$.

$$\theta = \frac{P_0}{8\sqrt{\pi\lambda}}\left\{\frac{1}{|z|^{1/2}}\exp[-x^2/4\lambda|z|]\right\} \tag{9}$$

$$\delta = \frac{P_0}{16\sqrt{\pi\lambda}}\left\{\frac{x}{|z|^{3/2}}\exp[-x^2/4\lambda|z|]\right\} \tag{10}$$

we see that both θ and δ fall off exponentially as we move along x.

b. Screw dislocations[15,14]

The dislocation line is along z-axis,

$$u = \frac{P_0}{4\pi}\alpha N \tag{11}$$

α is the polar angle $\tan^{-1}y/x$, and N an integer.

c. λ^+ and τ^+ disclinations

If **D** is the layer normal and the disclinations is along y, we find

$$\mathbf{D} = \begin{bmatrix}\cos\varphi \\ 0 \\ \sin\varphi\end{bmatrix} \qquad \begin{aligned}\varphi &= \alpha \quad \text{for} \quad \frac{\pi}{2} < \alpha < 3\frac{\pi}{2} \\ &= \frac{\pi}{2} \quad \text{for} \quad \frac{\pi}{2} > \alpha > 3\frac{\pi}{2}\end{aligned} \tag{12}$$

For λ^+ the central plane in the region $\varphi = \pi/2$ has its molecules along y, while for τ^+ it is along x.

3. RESULTS

We shall now consider the implications of the above theory. The edge dislocation solution Eq. (8) is very different from the nematic disclination solution Eq. (2). In fact, it is identical to the smectic A solution. The energy of the dislocation in an infinite medium is[15,14]

$$W \approx \frac{0.6\pi KP}{4\xi} \quad (K = K_{11} = K_{22} = K_{33}) \tag{13}$$

where ξ is the core radius. In this model it is of the order of $P_0/2$. This energy is finite and is quite different from $\frac{1}{4}\pi K \ln R/r_c$ (R being the sample size, r_c core size) suggested by Eq. (2) which diverges to ∞ as $R \to \infty$. Thus Eq. (8) appears to be energetically favorable. Another interesting consequence of Eq. (8) is that between two like dislocations one at (0,0) and another at (x_0, z_0), we have the forces F_x and F_z (along and perpendicular to the layers) acting between them, given by

$$\begin{aligned} F_x &= \frac{KP_0^2}{32\pi\lambda^2}\left(\frac{\pi}{\lambda}\right)^{1/2}\left(\frac{x_0}{z_0^{3/2}}\right)\exp[-x_0^2/4\lambda z_0] \\ F_z &= \frac{KP_0^2}{32\pi\lambda}\left(\frac{\pi}{\lambda}\right)^{1/2}\left(\frac{1}{z_0^{3/2}}\right)\left(1 - \frac{x_0^2}{2\lambda z_0}\right)\exp[-x_0^2/4\lambda z_0] \end{aligned} \tag{14}$$

F_x is always a repulsive force, while F_z is repulsive for $z_0 > x_0^2/2\lambda$ and attractive for $z_0 < x_0^2/2\lambda$. This results in a clustering of like-edge dislocations to form a low angle grain boundary. This appears to support the experimental observations of Bouligand and Kleman.[15] Again in a wedge one gets a minimum energy configuration of equally spaced [at distances $P_0/2$] like edge dislocations resulting in the Grandjean-Cano pattern.

In the case of screw dislocations described by Eq. (11) in terms of layer deformations, one can recast it to indicate changes in director orientation. One finds Eq. (11) to go over Eq. (1) which are similar to wedge disclinations in nematics. In smectic A, solutions Eq. (11) have no energies associated with them nor do disclinations interact. In cholesterics F is zero for this solution. However, F_0 is non-zero. In fact, we get the dislocation energies and interactions that we find in nematics. In this sense, screw disclinations in cholesterics are topologically equivalent to smectic A screw dislocations but energetically similar to nematic disclinations.

Finally, as regards their slow motions there is an interesting distinction between screw and edge dislocations. Elastic energy stored in the pattern

described by Eq. (1) or Eq. (2) is proportional to s^2 and this is dissipated as the pattern moves, resulting in a frictional force[16,17] proportional to s^2. However, edge dislocation motion in smectic A is akin to the familiar Stokes problem. It acts as an obstacle of size proportional to its Burgers vector resulting in a frictional force proportional to its Burgers vector, i.e. the strength itself.[18] Thus in this respect, also, there should be a marked difference between edge and screw dislocations in cholesterics.

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